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Discontinuous Galerkin Formulation for Multi-component Multiphase Flow

by

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ABSTRACT

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The understanding of multiphase multi-component transport in capillary porous media plays an important role in scientific and engineering disciplines such as the petroleum and environmental industries. The two most commonly used tools to model multiphase multi-component flow are finite difference and finite volume methods. While these are well-established methods, they either fail to provide stability on unstructured meshes or they yield low order approximation. In this thesis, a presentation of both fully coupled and sequential discontinuous Galerkin (DG) formulations for the multiphase multi-component flow is given. Two physical models are examined: the black oil model and the CO_2 sequestration model. The attractive attribute of using DG is that it permits the use of unstructured meshes while maintaining high order accuracy. Furthermore, the method can be structured to ensure mass conservation, which is another appealing feature when one is dealing with fluid dynamic problems.

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Chapter 1

Introduction

The study of multi-component multiphase flow is important in a wide range of industries. In this thesis, two new schemes are proposed to solve the fluid flow problems that arise in the petroleum and environmental disciplines. Both fully coupled and sequential numerical schemes are developed based on discontinuous Galerkin (DG) approximation. The model used to predict the black oil flow involve the compositional pressure and saturation equations developed by Watts ([10], 1986). This is a popular model used in the oil industry, however no work has been done to solve this model using the DG method. As for the CO_2 sequestration problem, there has been few investigations on the traditional model that uses DG. The advantage of these schemes is significant, as they retain high order approximations of pressures and saturations while conserving mass locally.

1.1 Motivation

The demand for energy is outpacing new discoveries of oil. In the year of 2009, the United States consumed approximately 20.7 million barrels of oil a day, which is a 3 million barrel a day increase in comparison to the year 1995. This motivates the need to model petroleum reservoir in order to develop optimum performance and strategies.

A petroleum reservoir is a porous medium where hydrocarbons are trapped inside the pore of a rock. Oil production in such reservoir is implemented in three phases: primary, secondary and tertiary recovery stage. In the primary recovery stage, oil can be easily extracted by relying on sufficient underground pressure in the reservoir. This pressure forces the oil to the surface; however, only an approximate of 10 percent of oil can be restored in this stage.

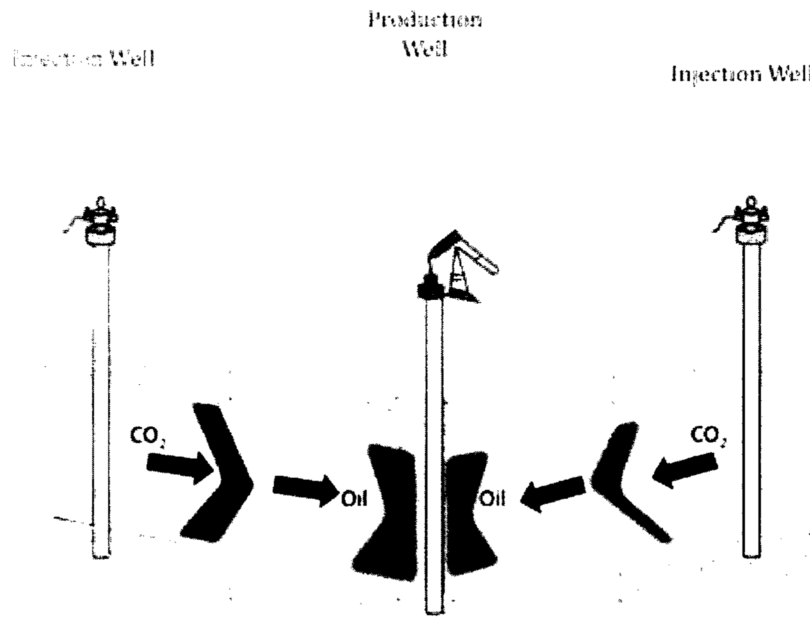

Figure 1.1 : Oil Recovery Process

In the secondary recovery, injection of fluids in wells is enforced. The well where fluids are injected into is called an injection well and it is used to facilitate oil production by increasing the pressure and flow rates of the reservoir. Oil is then extracted through another well called a production well (See Fig1.1). The recovery factor from this process is about 30-40 percent. In order to recover the remaining oil, companies turns to the tertiary recovery stage where more complex chemicals, for example

CO_2, are injected to the reservoir to increase the mobility of oil. Ongoing research on reservoir simulation are still being conducted to analyze and forecast fluid flows of the system.

In addition to the petroleum industry, an understanding of the multiphase flow in porous media also plays an important role in the environmental business. Major research projects are currently being performed on problems such as geological sequestration of carbon dioxide (CO_2). The alarming CO_2 greenhouse effect has been notably the number one cause of global warming on the planet. To address this problem, deep aquifers have been ubiquitously developed as a venue to trap large volumes of CO_2. A deep aquifer is a geological formation of permeable rocks built deep underground. On top of the aquifer, a cap rock is built to prevent CO_2 from escaping. However, the issue pertaining to the possibility of leakage of carbon dioxide remains. To ensure that the risk of leakage is minimized, an improved understanding of fluid flow and the response due to the change in fluid pressure is necessary.

1.2 Literature Search

To maximize the production of oil in a petroleum reservoir, many of the oil fields require the pressure to be kept above the bubble-point. Doing so keeps oil remaining in a single liquid phase in which helps avoid gas cap from forming in the pore space and helps stimulate the mobility of the fluid. Following the primary recovery stage, if the pressure falls below the bubble point, oil coexists in three phases: liquid, vapor and aqueous. Under these circumstances, oil is a multiphase multi-component mixture and the study of such a flow problem is important for oil reservoir simulation.

The black oil reservoir is a porous medium consisting of hydrocarbons. This reservoir is formed by a porous fractured rock and is located deep beneath the surface of the earth. In the petroleum industry, major efforts have been placed to better understand the flow in black oil reservoirs. The commonly used numerical methods for modeling multiphase flow in porous media include finite difference and finite volume methods. These two methods are well-established strategies (Douglas [3], Durlofsky [4]); however, while the finite difference method is straightforward to implement and efficient on standard structured grids, it exhibits instability on unstructured meshes. As for the finite volume methods, they are of low order.

Driven by the need for higher accuracy approximation, the discontinuous Galerkin (DG) method is employed (Reed and Hill [5]). The key stimulus for applying DG is due to the fact that an arbitrarily high order of accuracy can be obtained with a compact stencil. In addition, DG exhibits appealing features such as keeping mass locally conserved as well as having the ability to easily handle complex geometric domains. The study of two-phase flow in porous media has been successfully implemented and documented (Riviere and Bastian [6]), so it is only natural to extend this scheme to multi-phase multi-component flow.

While much work has been performed with DG methods for incompressible multiphase flow (Riviere [7], Natvig and Lie [8]), relatively few investigations have been done on multiphase flow that includes the effect of compressibility. Such an effect is important if the gas phase exists, as it does when the pressure is below the bubble point. In particular, gas has a relatively large compressibility; thus the consideration of it is important, as there can be a considerable spatial compressibility variation within the petroleum reservoir (Zhou and Tchelepi [9]).

The governing equation of the multiphase multi-component flow in porous media is given by the pressure-saturation equation. Existing solution techniques used to solve for this system of equations includes implicit pressure-explicit saturation (IMPES) and the coupled implicit method. With the IMPES framework, the pressure equation is computed implicitly with the remaining equations being evaluated explicitly. This algorithm leads to a relatively fast solution in terms of time step basis; however, the time step size is greatly limited by the imposed stability constraints (Watts [10], pp. 243). On the other hand, the coupled implicit technique does not encounter any stability issues; nevertheless, this method becomes rapidly uneconomical as we increase the size of the model.

To include both robustness and stabilization of the system, Watts developed a method called the sequential implicit procedure (Watts [10]). In particular, the sequential implicit procedure employs IMPES to determine the pressure and uses implicit treatment to solve for the saturation. Furthermore, it was shown that when black oil fluid properties are applied, the formulation reduces back to the conventional black oil equation. Besides the attractive feature to easily change the compositional model back to the black oil model, this formulation reveals a meaningful physical phenomenon of the system. That is, the pressure equation represents the volume balance (Acs et al. [11]).

This thesis presents two different approaches to solve the pressure-saturation problem for multiphase flow based on the pressure-saturation formulation developed by Watts. One is the DG method with the fully coupled approach and the other is the DG method with the sequential approach. In both approaches, the model utilizes DG for spatial discretization. In regard to the fully coupled approach, the coupled system of nonlinear equations is solved by applying an iterative scheme, namely Newton-Raphson. The advantage of this scheme is that it does not require slope limiters or upwinding stabilization techniques. As for the sequential approach, the pressure and saturation equations are decoupled and solved sequentially by time lagging the coefficients, whereas the saturations equations are solved successively. This method provides efficient solutions while eradicating the non-linearity difficulty.

Besides solving the black oil model (Watts [10]), a numerical scheme for the geological sequestration of carbon dioxide (CO_2) is developed as well. The traditional multiphase flow model, TOUGH2, neglected the effect of triple point temperature as well as the various states of the CO_2 fluid (Pruess [12]), specifically the supercritical state. In efforts to incorporate these conditions, a joint work including Sasaki, Fujii, Niibori, Ito and Hashida developed a model based on the usage of equation of state for CO_2 established by Span and Wagner to include the CO_2 density (Sasaki et al. [13], Span and Wagner [14]). Furthermore, to account for the CO_2 dissolution in water, Sasaki proposed to take mole fractions of each component phase into consideration when dealing with the flux term and has noted that the mole fractions of CO_2 can be calculated using Henrys law (Sasaki et al. [13],pp.47-48).

Using the Sasaki formulation model of the pressure-saturation equations, a scheme based on discontinuous approximation spaces is established for solving this system. Noting that the obtained system is a function of the mole fractions of water in vapor and aqueous phase, the fugacity equation mentioned by Spycher and Pruess is exploited for the computation of the corresponding mole fractions (Spycher and Pruess [15]).

1.3 Plan of Thesis

This thesis is composed of four chapters. Chapter 2 presents a brief background on both the saturated black oil model and the CO_2 sequestration model following an outline of the assumptions for the data. A presentation of the compositional formulation of the pressure and saturation equations is given in detail.

Chapter 3 is the heart of this work, in this chapter we will use the resulting pressure-saturation formulation developed in Chapter 2 to formulate two new schemes to solve the compressible multiphase multi-component flow in porous media. I first present the sequential approach where the coupled pressure and saturations equations are linearized and solve sequentially by time-lagging all the nonlinear coefficients. Then I present the fully coupled approach where the resulting pressure and saturations system are decoupled by Newton-Raphson method. A backward Euler technique is used for the time discretization.

Conclusions and a discussion of future possible approaches are presented in Chapter 4. Finally, Chapter 5 provides the definitions to the notations used throughout the thesis.

Chapter 2

Mathematical Model

This chapter presents the compositional formulation of the pressure and saturation equations for both the black oil and CO_2 sequestration model. Based on the preliminary equations developed here, two numerical discontinuous Galerkin schemes are established in the following chapter. For the black oil model, the basic equations for multicomponent multiphase flow are written as a set of one pressure equation and two saturation equations (Watts [10]). As for the CO_2 sequestration model, a set of one pressure equation and one saturation equation are used to describe its flow.

First an introduction of the black oil model is given. This model have three phases: liquid (L), vapor (v), aqueous (a) and three components: oil (o), gas (g), water (w). It is assumed that the aqueous phase does not exchange mass with liquid or vapor phase. The liquid and vapor phases do exchange mass. Here are the underlying assumptions of the data.

2.1 Assumptions

1. The primary variable is $p := p_L$, the pressure of the liquid phase.

2. Capillary pressure correspond to the differences in pressure between the interface of phases and it is given by:

$$p_{ca} = p_a - p, \tag{2.1}$$

$$p_{cv} = p_v - p. \tag{2.2}$$

3. Both p_{ca} and p_{cv} are functions of saturations: $p_{ca} = p_{ca}(S_a), \quad p_{cv} = p_{cv}(S_v)$.

4. Relative permeabilities for water and gas are functions of saturations:

$$k_{ra} = k_{ra}(S_a), \quad k_{rv} = k_{rv}(S_v), \quad k_{rL} = k_{rL}(S_a, S_v).$$

5. Vicosities for oil and gas are functions of pressure: $\mu_L = \mu_L(p), \quad \mu_v = \mu_v(p)$.

6. Volume formation factor for oil and gas (B_L, B_v) can be used to describe the reduction of oil and gas respectively as it is being brought to the surface. It is defined as

$$B_\alpha = \frac{V_\alpha^R}{V_\alpha^S}, \quad \text{for } \alpha = L, v \tag{2.3}$$

where V_α^R is the volume in phase α at reservoir conditions and V_α^S is the volume in phase α at standard conditions. It is assumed to be a function of pressure: $B_L = B_L(p), \quad B_v = B_v(p)$.

7. Solution gas/liquid ratio (R_{sL}) is the ratio of the volume of produced gas to the volume of produced liquid and it is function of pressure: $R_{sL} = R_{sL}(p)$.

8. Compressibility of phase α are function of pressure: $c_\alpha = c_\alpha(p)$.

9. Density in phase α are function of pressure: $\rho_\alpha = \rho_\alpha(p)$.

2.2 Saturated Black-Oil Model

Assuming that the temperature is constant, the pressure equation for the pressure is given by ($p = p_L$ for instance):

$$\left(\frac{d\phi}{dp} - \frac{\phi}{\nu_T} \left(\frac{\partial \nu_T}{\partial p} \right)_z \right) \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m \tag{2.4}$$

Second for each phase α the saturation equation is:

$$\frac{\partial}{\partial t}(\phi S_\alpha) = -\phi S_\alpha c_\alpha \frac{\partial p}{\partial t} + \sum_m V_{\alpha m}\Theta_m \tag{2.5}$$

where

- Porosity ϕ is the measure of the pore space of the rock. It is defined to be the ratio of the volume of pores to the total volume. i.e.

$$\phi = \frac{V_{\text{pore}}}{V_{\text{total}}} \tag{2.6}$$

  where V stands for volume.

- Specific volume ν_α of phase α is the reciprocal of the mass density. That is, the fraction of mass in phase α to the volume in phase α, which is given by

$$\nu_\alpha = \frac{m_\alpha}{V_\alpha}. \tag{2.7}$$

  and the total specific volume is defined to be $\nu_T = \sum_\alpha \nu_\alpha$. In the term $-\frac{\phi}{\nu_T}\left(\frac{\partial \nu_T}{\partial p}\right)_z$, z represents the overall mole fraction.

- Partial molar volume $V_{\alpha m}$ is the derivative of the volume in phase α with respect to the number of moles in component m. It can be expressed as

$$V_{\alpha m} = \frac{\partial V_\alpha}{\partial N_m}, \tag{2.8}$$

  where N_m represents the total number of moles in component m. Therefore, in (2.4) , $V_{Tm} = \frac{\partial V_T}{\partial N_m}$ where V_T stands for total volume.

- Divergence of the flux of component m is denoted as Θ_m.

- Saturation S_α of phase α is the fraction of the volume in phase α that fills the total pore space and it is given by

$$S_\alpha = \frac{V_\alpha}{V_{\text{pore}}}. \tag{2.9}$$

From (Watts [10]), we obtain the partial molar volumes and phase compressibilities:

$$V_{Lo} = B_L, \quad V_{Lg} = V_{Lw} = 0 \tag{2.10}$$

$$V_{vo} = -B_v R_{sL}, \quad V_{vg} = B_v, \quad V_{vw} = 0 \tag{2.11}$$

$$V_{ao} = V_{ag} = 0, \quad V_{aw} = B_a \tag{2.12}$$

$$c_L = -\frac{1}{B_L}\frac{\partial B_L}{\partial p} \tag{2.13}$$

$$c_v = -\frac{1}{B_v}\frac{\partial B_v}{\partial p} + \frac{S_L B_v}{S_v B_L}\frac{\partial R_{sL}}{\partial p} \tag{2.14}$$

$$c_a = -\frac{1}{B_a}\frac{\partial B_a}{\partial p} \tag{2.15}$$

Note that B_L, B_a, B_v, R_{sL} are known functions of pressure p and the fluxes Θ_m are functions of both pressure and saturation. Let $\boldsymbol{u}_\alpha$ denote the velocity of phase α. Then from Darcy's law, we have:

$$\boldsymbol{u}_\alpha = -\frac{k_{r\alpha}\mathbf{k}}{\mu_\alpha}\nabla(p_\alpha - \rho_\alpha g D), \tag{2.16}$$

where $k_{r\alpha}$ is the relative permeability for phase α, $\mathbf{k}$ is the absolute permeability tensor of the porous medium, μ_α is the fluid viscosity of phase α, D is the depth of the reservoir and g is the gravitational constant (Chen [16]). Then, we have

$$\Theta_w = -\nabla \cdot \left(\frac{\boldsymbol{u}_a}{B_a}\right), \tag{2.17}$$

$$\Theta_o = -\nabla \cdot \left(\frac{\boldsymbol{u}_L}{B_L}\right), \tag{2.18}$$

$$\Theta_g = -\nabla \cdot \left(\frac{\boldsymbol{u}_v}{B_v} + R_{sL}\frac{\boldsymbol{u}_L}{B_L}\right). \tag{2.19}$$

Define

$$\alpha_r = \frac{k_{r\alpha}\mathbf{k}}{\mu_r}. \tag{2.20}$$

With the definition of (2.20), we now compute the divergence of flux of each component from (2.16), (2.17), (2.18), (2.19).

Divergence Flux of Water Component

$$\begin{aligned}
\Theta_w &= -\nabla\cdot\Big(-\frac{\alpha_a}{B_a}\nabla(p_a-\rho_a gD)\Big)\\
&= \nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_a\Big)-\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla(\rho_a gD)\Big)\\
&= \nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p\Big)+\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_{ca}\Big)-\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla(\rho_a gD)\Big)
\end{aligned}\tag{2.21}$$

Divergence Flux of Oil Component

$$\begin{aligned}
\Theta_o &= -\nabla\cdot\Big(-\frac{\alpha_L}{B_L}\nabla(p-\rho_L gD)\Big)\\
&= \nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla p\Big)-\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\Big)
\end{aligned}\tag{2.22}$$

Divergence Flux of Gas Component

$$\begin{aligned}
\Theta_g &= -\nabla\cdot\frac{\boldsymbol{u}_v}{B_v}-\nabla\cdot\Big(R_{sL}\frac{\boldsymbol{u}_L}{B_L}\Big)\\
&= \nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_v\Big)-\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla(\rho_v gD)\Big)+\nabla\cdot\Big(R_{sL}\frac{\alpha_L}{B_L}\nabla p_L\Big)\\
&\quad -\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\Big)\\
&= \nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p\Big)+\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_{cv}\Big)-\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla(\rho_v gD)\Big)\\
&\quad +\nabla\cdot\Big(R_{sL}\frac{\alpha_L}{B_L}\nabla p_L\Big)-\nabla\cdot\Big(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\Big)
\end{aligned}\tag{2.23}$$

It remains to define the terms in the pressure equation. Note that the rock compressibility c_R is given by

$$c_R=\frac{1}{\phi}\frac{\partial\phi}{\partial p}.\tag{2.24}$$

Integrating (2.24) yields

$$\phi=\phi^o e^{c_R(p-p^o)},\tag{2.25}$$

where p^o is the reference pressure and ϕ^o is the porosity at p^o. Applying Taylor expansion, one arrives at

$$\phi=\phi^o\Big(1+c_R(p-p^o)+\frac{c_R^2(p-p^o)^2}{2!}+\cdots\Big).\tag{2.26}$$

This yields an approximation:

$$\phi \approx \phi^o(1 + c_R(p - p^o)). \tag{2.27}$$

We next compute the total compressibility $\frac{1}{\nu_T}(\frac{\partial \nu_T}{\partial p})_z$ with z as the overall mole fraction. From $\nu_T = \nu_L + \nu_a + \nu_v$ we have

$$\frac{\partial \nu_T}{\partial p} = \frac{\partial \nu_L}{\partial p} + \frac{\partial \nu_a}{\partial p} + \frac{\partial \nu_v}{\partial p}. \tag{2.28}$$

The compressibility of phase α can be expressed as

$$c_\alpha = -\frac{1}{\nu_\alpha}\left(\frac{\partial \nu_\alpha}{\partial p}\right)_z, \tag{2.29}$$

then,

$$-\frac{1}{\nu_T}\left(\frac{\partial \nu_T}{\partial p}\right)_z = \frac{\nu_L}{\nu_T}c_L + \frac{\nu_v}{\nu_T}c_v + \frac{\nu_a}{\nu_T}c_a. \tag{2.30}$$

Now notice that we can write

$$\frac{\nu_\alpha}{\nu_T} = \frac{V_\alpha}{V_T}\left(\frac{V_\alpha}{\nu_\alpha}\frac{\nu_T}{V_T}\right)^{-1} = S_\alpha\left(\frac{N_\alpha}{N_T}\right)^{-1} \tag{2.31}$$

as $V_\alpha = N_\alpha \nu_\alpha$ and $V_T = N_T \nu_T$. Thus we obtain,

$$-\frac{1}{\nu_T}\left(\frac{\partial \nu_T}{\partial p}\right)_z = c_L S_L\left(\frac{N_L}{N_T}\right)^{-1} + c_v S_v\left(\frac{N_v}{N_T}\right)^{-1} + c_a S_a\left(\frac{N_a}{N_T}\right)^{-1}. \tag{2.32}$$

From (Watts [10], pp. 248), we have

$$N_o = \frac{V_L}{B_L}, \quad N_g = \frac{V_v}{B_v} + \frac{V_L R_{sL}}{B_L}, \quad N_w = \frac{V_a}{B_a} \tag{2.33}$$

and we know that

$$N_T = N_o + N_w + N_g = N_L + N_a + N_v, \tag{2.34}$$

where N_m represents the number of moles in component $m \in \{o, w, g\}$ and N_α represents the number of moles in phase $\alpha \in \{L, a, v\}$. Since water does not exchange mass, we obtain

$$N_a = N_w, \quad N_v = \frac{V_v}{B_v}, \quad N_L = \frac{V_L}{B_L} + \frac{V_L R_{sL}}{B_L}. \tag{2.35}$$

Using the relation given above we can obtain the mass fractions as function of saturations and pressure:

$$\begin{aligned}
\frac{N_T}{N_a} &= \frac{1}{N_a}\left(\frac{V_L}{B_L} + \frac{V_L R_{sL}}{B_L} + N_a + \frac{V_v}{B_v}\right) \\
&= \frac{B_a}{V_a}\left(\frac{V_L}{B_L} + \frac{V_L R_{sL}}{B_L} + \frac{V_a}{B_a} + \frac{V_v}{B_v}\right) \\
&= \frac{B_a}{B_L}\frac{S_L}{S_a} + \frac{R_{sL} B_a}{B_L}\frac{S_L}{S_a} + 1 + \frac{B_a}{B_v}\frac{S_v}{S_a} \\
&= 1 + \frac{B_a S_L}{B_L S_a} + \frac{B_a}{S_a}\left(\frac{S_v}{B_v} + \frac{S_L R_{sL}}{B_L}\right),
\end{aligned} \tag{2.36}$$

and

$$\begin{aligned}
\frac{N_T}{N_v} &= \frac{1}{N_v}\left(\frac{V_L}{B_L} + \frac{V_L R_{sL}}{B_L} + \frac{V_a}{B_a} + N_v\right) \\
&= 1 + \frac{B_v}{V_v}\left(\frac{V_L}{B_L} + \frac{V_L R_{sL}}{B_L} + \frac{V_a}{B_a}\right) \\
&= 1 + \frac{B_v}{B_L}\frac{S_L V_T}{S_v V_T} + \frac{R_{sL} B_v}{B_L}\frac{S_L V_T}{S_v V_T} + \frac{B_v}{B_a}\frac{S_a V_T}{S_v V_T} \\
&= 1 + \frac{B_v R_{sL} S_L}{B_L S_v} + \frac{B_v S_a}{B_a S_v} + \frac{S_L B_v}{B_L S_v},
\end{aligned} \tag{2.37}$$

and

$$\begin{aligned}
\frac{N_T}{N_L} &= \frac{1}{N_L}\left(N_L + \frac{V_a}{B_a} + \frac{V_v}{B_v}\right) \\
&= 1 + \frac{B_L}{V_L(1 + R_{sL})}\left(\frac{V_a}{B_a} + \frac{V_v}{B_v}\right) \\
&= 1 + \frac{1}{1 + R_{sL}}\left(\frac{B_L}{B_a}\frac{S_a V_T}{S_L V_T} + \frac{B_L}{B_v}\frac{S_v V_T}{S_L V_T}\right) \\
&= (1 + R_{sL})^{-1}\left(1 + R_{sL} + \frac{S_a B_L}{B_a S_L} + \frac{S_v B_L}{B_v S_L}\right).
\end{aligned} \tag{2.38}$$

Note that the total partial molar volume is given by:

$$V_{Tm} = \frac{dV_T}{dN_m} = V_{Lm} + V_{vm} + V_{am}, \tag{2.39}$$

so from (2.10), (2.11), (2.12), we obtain

$$\begin{aligned} V_{To} &= V_{Lo} + V_{vo} + V_{ao} = B_L - B_v R_{sL}, & (2.40)\\ V_{Tg} &= V_{Lg} + V_{vg} + V_{ag} = B_v, & (2.41)\\ V_{Tw} &= V_{Lw} + V_{vw} + V_{aw} = B_a. & (2.42) \end{aligned}$$

From (2.21), (2.22), (2.23), we can rearrange the right-hand side of the pressure equation with the following form:

$$\begin{aligned} \sum_m V_{Tm}\Theta_m &= V_{To}\nabla\cdot(\frac{\alpha_L}{B_L}\nabla p) + V_{Tg}\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla p\right) + V_{Tw}\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla p\right)\\ &\quad + V_{Tg}\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla p_{cv}\right) + V_{Tg}\nabla\cdot\left(\frac{R_{sL}\alpha_L}{B_L}\nabla p\right) + V_{Tw}\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla p_{ca}\right) + X\\ &= (B_L - B_v R_{sL})\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla p\right) + B_v\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla p\right) + B_v\nabla\cdot(\frac{R_{sL}\alpha_L}{B_L}\nabla p)\\ &\quad + B_a\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla p\right) + B_v\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla p_{cv}\right) + B_a\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla p_{ca}\right) + X \end{aligned} \tag{2.43}$$

The function $X = X(p, S_a, S_L)$ contains the gravity terms:

$$\begin{aligned} X &= -V_{To}\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\right) - V_{Tg}\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla(\rho_v gD)\right)\\ &\quad - V_{Tw}\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla(\rho_a gD)\right) - V_{Tg}\nabla\cdot\left(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\right)\\ &= -(B_L - B_v R_{sL})\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\right) - B_v\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla(\rho_v gD)\right)\\ &\quad - B_a\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla(\rho_a gD)\right) - B_v\nabla\cdot\left(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L gD)\right) \end{aligned} \tag{2.44}$$

From (2.27), (2.32),(2.36), (2.37) ,(2.38), the left-hand side of the pressure equation

(2.4) becomes:

$$\begin{aligned}
\Big(\frac{d\phi}{dp} - \frac{\phi}{\nu_T}(\frac{\partial \nu_T}{\partial p})_z\Big)\frac{\partial p}{\partial t} &= \Big(\phi^o c_R + \phi^o(1 + c_R(p-p^o))\Big(c_L S_L\Big(\frac{N_L}{N_T}\Big)^{-1} + c_v S_v\Big(\frac{N_v}{N_T}\Big)^{-1} \\
&\quad + c_a S_a\Big(\frac{N_a}{N_T}\Big)^{-1}\Big)\Big)\frac{\partial p}{\partial t} \\
&= \Big(\phi^o c_R + \phi^o(1 + c_R(p-p^o)) \\
&\quad \Big(c_L S_L(1+R_{sL})^{-1}\Big(1 + R_{sL} + \frac{S_a B_L}{B_a S_L} + \frac{S_v B_L}{B_v S_L}\Big) \\
&\quad + c_v S_v\Big(1 + \frac{B_v R_{sL} S_L}{B_L S_v} + \frac{B_v S_a}{B_a S_v} + \frac{S_L B_v}{B_L S_v}\Big) \\
&\quad + c_a S_a\Big(1 + \frac{B_a S_L}{B_L S_a} + \frac{B_a}{S_a}\Big(\frac{S_v}{B_v} + \frac{S_L R_{sL}}{B_L}\Big)\Big)\Big)\frac{\partial p}{\partial t} \qquad (2.45)
\end{aligned}$$

The pressure equation in terms of $p, B_L, B_a, B_v, R_{SL}, S_v, S_a$ is given by:

Pressure Equation

$$\begin{aligned}
&\Big(\phi^o c_R + \phi^o(1 + c_R(p-p^o))\Big(c_L S_L(1+R_{sL})^{-1}\Big(1 + R_{sL} + \frac{S_a B_L}{B_a S_L} + \frac{S_v B_L}{B_v S_L}\Big) \\
&+ c_v S_v\Big(1 + \frac{B_v R_{sL} S_L}{B_L S_v} + \frac{B_v S_a}{B_a S_v} + \frac{S_L B_v}{B_L S_v}\Big) + c_a S_a\Big(1 + \frac{B_a S_L}{B_L S_a} + \frac{B_a}{S_a}\Big(\frac{S_v}{B_v} + \frac{S_L R_{sL}}{B_L}\Big)\Big)\Big)\Big)\frac{\partial p}{\partial t} \\
&= (B_L - B_v R_{sL})\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla p\Big) + B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p\Big) + B_v\nabla\cdot\Big(\frac{R_{sL}\alpha_L}{B_L}\nabla p\Big) \\
&+ B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p\Big) + B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_{cv}\Big) + B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_{ca}\Big) \\
&- (B_L - B_v R_{sL})\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\Big) - B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla(\rho_v g D)\Big) \\
&- B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla(\rho_a g D)\Big) - B_v\nabla\cdot\Big(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\Big) \qquad (2.46)
\end{aligned}$$

Now let us rewrite the right-hand side of the saturation equation (2.5). Using (2.10), (2.13), (2.22) we have

Saturation Equation for phase L

$$\begin{aligned}
\frac{\partial}{\partial t}(\phi S_L) &= -\phi S_L\left(-\frac{1}{B_L}\frac{\partial B_L}{\partial p}\right)\frac{\partial p}{\partial t} + V_{Lo}\Theta_o + V_{Lg}\Theta_g + V_{Lw}\Theta_w \\
&= -\phi S_L\left(-\frac{1}{B_L}\frac{\partial B_L}{\partial p}\right)\frac{\partial p}{\partial t} + B_L\Theta_o \\
&= -\phi S_L\left(-\frac{1}{B_L}\frac{\partial B_L}{\partial p}\right)\frac{\partial p}{\partial t} + B_L\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla p\right) \\
&\quad -B_L\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\right) \qquad (2.47)
\end{aligned}$$

By (2.11) and (2.14), we obtain:

Saturation Equation for phase v

$$\begin{aligned}
\frac{\partial}{\partial t}(\phi S_v) &= -\phi S_v\left(-\frac{1}{B_v}\frac{\partial B_v}{\partial p} + \frac{S_L}{S_v}\frac{B_v}{B_L}\frac{\partial R_{sL}}{\partial p}\right)\frac{\partial p}{\partial t} + V_{vo}\Theta_o + V_{vg}\Theta_g + V_{vw}\Theta_w \\
&= -\phi S_v\left(-\frac{1}{B_v}\frac{\partial B_v}{\partial p} + \frac{S_L}{S_v}\frac{B_v}{B_L}\frac{\partial R_{sL}}{\partial p}\right)\frac{\partial p}{\partial t} - B_v R_{sL}\Theta_o + B_v\Theta_g \\
&= -\phi S_v\left(-\frac{1}{B_v}\frac{\partial B_v}{\partial p} + \frac{S_L}{S_v}\frac{B_v}{B_L}\frac{\partial R_{sL}}{\partial p}\right)\frac{\partial p}{\partial t} \\
&\quad -B_v R_{sL}\left(\nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla p\right) - \nabla\cdot\left(\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\right)\right) \\
&\quad +B_v\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla(p_{cv}+p)\right) - B_v\nabla\cdot\left(\frac{\alpha_v}{B_v}\nabla(\rho_v g D)\right) \\
&\quad +B_v\nabla\cdot\left(R_{sL}\frac{\alpha_L}{B_L}\nabla p\right) - B_v\nabla\cdot\left(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\right) \qquad (2.48)
\end{aligned}$$

Now from (2.12) and (2.15), one arrive at:

Saturation Equation for phase a

$$\begin{aligned}
\frac{\partial}{\partial t}(\phi S_a) &= -\phi S_a\left(-\frac{1}{B_a}\frac{\partial B_a}{\partial p}\right)\frac{\partial p}{\partial t} + V_{ao}\Theta_o + V_{ag}\Theta_g + V_{aw}\Theta_w \\
&= -\phi S_a\left(-\frac{1}{B_a}\frac{\partial B_a}{\partial p}\right)\frac{\partial p}{\partial t} + B_a\Theta_w \\
&= -\phi S_a\left(-\frac{1}{B_a}\frac{\partial B_a}{\partial p}\right)\frac{\partial p}{\partial t} + B_a\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla(p_{ca}+p)\right) \\
&\quad -B_a\nabla\cdot\left(\frac{\alpha_a}{B_a}\nabla(\rho_a g D)\right) \qquad (2.49)
\end{aligned}$$

2.3 CO_2 sequestration Model

Carbon dioxide disposal into deep aquifer has been an important venue to trap excess gas emission, not only is this technology economical, it provides a promising media to trap large capacity of residual gas. In the CO_2 sequestration process, we have two components (i.e. CO_2 and H_2O) and two phases (i.e. liquid (L) and vapor (v) phase). The mathematical model of this compositional problem can be described by a set of mass conservation equations and thermodynamic equilibrium formulae (Voskov et al. [17]). Specifically, the conservation equations used to describe the transport phenomenon of the fluid are established by Sasaki to account for the CO_2 dissolution effect into water (Sasaki et al. [13]). The transport equations for the multiphase multicomponent flow in porous media is given by:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\phi(x_{CO_2,L}\rho_L S_L + x_{CO_2,v}\rho_v S_v)\right) + \nabla\cdot\left(x_{CO_2,L}\rho_L \boldsymbol{u}_L + x_{CO_2,v}\rho_v \boldsymbol{u}_v\right)\\
&+x_{CO_2,L}\rho_L q_L + x_{CO_2,v}\rho_v q_v = 0, \qquad (2.50)\\
&\frac{\partial}{\partial t}\left(\phi(x_{H_2O,L}\rho_L S_L + x_{H_2O,v}\rho_v S_v)\right) + \nabla\cdot\left(x_{H_2O,L}\rho_L \boldsymbol{u}_L + x_{H_2O,v}\rho_v \boldsymbol{u}_v\right)\\
&+x_{H_2O,L}\rho_L q_L + x_{H_2O,v}\rho_v q_v = 0. \qquad (2.51)
\end{aligned}$$

Here $x_{m,\alpha}$ is the mole fraction of component m in phase α, $\boldsymbol{u}_\alpha$ is the phase velocity of phase α defined in (2.16) but neglecting the effect of gravity and q_α is the source term of phase α. In addition, we have the capillary pressure p_{cv} defined by (2.2). The state of thermodynamic equilibrium are given by:

$$f_{CO_2,L}(p,T,x_{CO_2,L}) - f_{CO_2,v}(p,T,x_{CO_2,v}) = 0 \qquad (2.52)$$

$$f_{H_2O,L}(p,T,x_{H_2O,L}) - f_{H_2O,v}(p,T,x_{H_2O,v}) = 0 \qquad (2.53)$$

Here we denote p as the liquid phase pressure and $f_{m,\alpha}$ as the fugacity of component m in phase α. Fugacity is a thermodynamic property that describes the tendency of a gas to escape.

Phase constraint:

$$x_{CO_2,L} + x_{H_2O,L} = 1 \tag{2.54}$$

$$x_{CO_2,v} + x_{H_2O,v} = 1 \tag{2.55}$$

Saturation constraint:

$$S_L + S_v = 1 \tag{2.56}$$

Inserting (2.2), (2.16)and (2.56) into (2.50) and (2.51) yields:

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\phi^o(1 + c_R(p - p^o))(x_{CO_2,L}\rho_L S_L + x_{CO_2,v}\rho_v(1 - S_L))\right) \\
&-\nabla \cdot \left(x_{CO_2,L}\rho_L\alpha_L\nabla p + x_{CO_2,v}\rho_v\alpha_v\nabla(p_{cv} + p)\right) \\
&+x_{CO_2,L}\rho_L q_L + x_{CO_2,v}\rho_v q_v = 0,
\end{aligned} \tag{2.57}$$

and

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\phi^o(1 + c_R(p - p^o))(x_{H_2O,L}\rho_L S_L + x_{H_2O,v}\rho_v(1 - S_L))\right) \\
&-\nabla \cdot \left(x_{H_2O,L}\rho_L\alpha_L\nabla p + x_{H_2O,v}\rho_v\alpha_v\nabla(p_{cv} + p)\right) \\
&+x_{H_2O,L}\rho_L q_L + x_{H_2O,v}\rho_v q_v = 0,
\end{aligned} \tag{2.58}$$

The model above is a closed system for the CO_2 sequestration processes. Next we consider the fugacity equations. It has been suggested that we can solve this by solving the mole fraction of water in CO_2 in vapor and aqueous phase (Spycher [15]). Then we can obtain the expression:

$$x_{H_2O,v} = \frac{K_{H_2O,T,p^o} \cdot (1 - x_{CO_2,L})}{\tau_{H_2O} \cdot p} \cdot exp\left(\frac{(p - p^o) \cdot \bar{V}_{H_2O}}{RT}\right), \tag{2.59}$$

$$x_{CO_2,L} = \frac{\tau_{CO_2} \cdot (1 - x_{H_2O,v}) \cdot p}{K_{CO_2,T,p^o} \cdot 55.508} \cdot exp\left(-\frac{(p - p^o) \cdot \bar{V}_{CO_2}}{RT}\right), \tag{2.60}$$

where τ_m is the fugacity coefficient of component m, $K_{m,t,p}$ is the thermodynamic equilibrium constant of component m at temperature t and pressure p, $\bar{V}_m$ is the average partial molar volume of component m and R is the gas constant with

$$K_{H_2O,T,P} = \frac{f_{H_2O,v}}{1 - x_{CO_2,L}} \tag{2.61}$$

$$K_{CO_2,T,P} = \frac{f_{CO_2,v}}{55.508 x_{CO_2,L}} \tag{2.62}$$

For simplicity, we can denote

$$A = \frac{K_{H_2O,T,P^o}}{\tau_{H_2O} p} exp\left(\frac{(p - p^o)\overline{V}_{H_2O}}{RT}\right), \tag{2.63}$$

$$B = \frac{\tau_{CO_2} P}{55.508 K_{CO_2,T,p^o}} exp\left(-\frac{(p - p^o)\overline{V}_{CO_2}}{RT}\right). \tag{2.64}$$

Hence,

$$x_{H_2O,v} = \frac{1 - B}{(1/A) - B}, \tag{2.65}$$

$$x_{CO_2,L} = B(1 - x_{H_2O,v}) \tag{2.66}$$

Fugacity coefficients of CO_2 can be obtained from curves in Fig 2.1, where τ_{CO_2} at each specific temperature under various pressure is given.

In the next chapter, we develop a system of differential equations for both the black oil model and CO_2 sequestration model by utilizing the equations developed here and establish a DG scheme to solve the system.

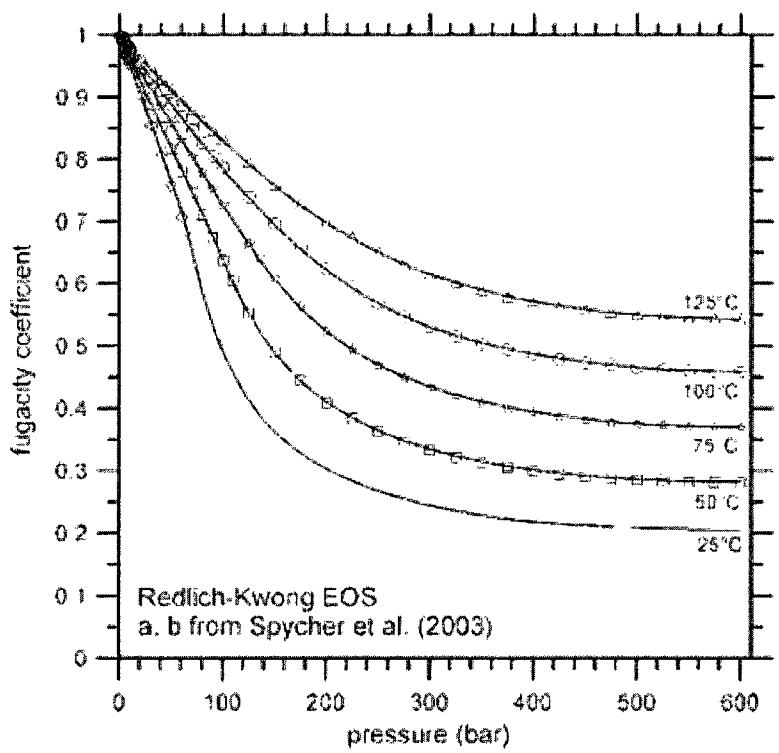

Figure 2.1 : Fugacity coefficient of CO_2 at 25, 50, 74, 100 and 125^{o}C under different values of pressures (Marini [1], p. 37)

Chapter 3

DG Formulation

In this chapter, a formulation of the discontinuous Galerkin scheme of the multiphase multi-component is established. Here, we focus exclusively on the saturated black oil model and the CO_2 sequestration model. Two approaches are developed to solve the pressure-saturation formulations of the black oil model as well as the transport equations of the CO_2 sequestration model. One approach is obtained by decoupling the solution of the equations and solving them sequentially. The other approach solves the discretized system using a fully implicit scheme, where the Jacobian matrix is computed at each time step.

3.1 Sequential Formulation for Saturated Black Oil Model

Here we present one possible technique which is to solve for pressure first by time-lagging the coefficients, then for saturations. The primary unknowns are the liquid phase pressure p, the liquid phase saturation S_L and the aqueous phase saturation S_a. Discretizing (2.46), (2.47), (2.49) in time, we obtain the following equations:

Pressure Equation

$$\Big(\phi^o c_R + \phi^o(1 + c_R(p - p^o))\Big)\Big(c_L S_L (1 + R_{sL})^{-1}\Big(1 + R_{sL} + \frac{S_a B_L}{B_a S_L} + \frac{S_v B_L}{B_v S_L}\Big)$$
$$+c_v S_v\Big(1 + \frac{B_v R_{sL} S_L}{B_L S_v} + \frac{B_v S_a}{B_a S_v} + \frac{S_L B_v}{B_L S_v}\Big)$$
$$+c_a S_a\Big(1 + \frac{B_a S_L}{B_L S_a} + \frac{B_a}{S_a}\Big(\frac{S_v}{B_v} + \frac{S_L R_{sL}}{B_L}\Big)\Big)\Big)\Big)^n \frac{p^{n+1} - p^n}{\Delta t}$$
$$-\Big((B_L - B_v R_{sL})\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla p^{n+1}\Big) + B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p^{n+1}\Big) + B_v\nabla\cdot\Big(\frac{R_{sL}\alpha_L}{B_L}\nabla p^{n+1}\Big)$$
$$+B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p^{n+1}\Big) + B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_{cv}\Big) + B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_{ca}\Big)$$
$$-(B_L - B_v R_{sL})\nabla\cdot\Big(\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\Big) - B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla(\rho_v g D)\Big)$$
$$-B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla(\rho_a g D)\Big) - B_v\nabla\cdot\Big(R_{sL}\frac{\alpha_L}{B_L}\nabla(\rho_L g D)\Big)\Big)^n = 0 \qquad (3.1)$$

Saturation Equation for phase L

$$\frac{1}{\Delta t}((\phi S_L)^{n+1} - (\phi S_L)^n) + \left(\phi S_L\left(-\frac{1}{B_L}\frac{dB_L}{dp}\right)\right)^{n+1}\frac{p^{n+1} - p^n}{\Delta t}$$
$$-B_L^{n+1}\left(\nabla\cdot\left(\frac{\alpha_L^n}{B_L^{n+1}}\nabla p^{n+1}\right) - \nabla\cdot\left(\frac{\alpha_L^n}{B_L^{n+1}}\nabla(\rho_L^{n+1} g D)\right)\right) = 0 \qquad (3.2)$$

Saturation Equation for phase a

$$\frac{1}{\Delta t}((\phi S_a)^{n+1} - (\phi S_a)^n) + \left(\phi S_a\left(-\frac{1}{B_a}\frac{dB_a}{dp}\right)\right)^{n+1}\frac{p^{n+1} - p^n}{\Delta t}$$
$$-B_a^{n+1}\left(\nabla\cdot\left(\frac{\alpha_a^n}{B_a^{n+1}}\nabla(p_{ca}^{n+1} + p^{n+1})\right) - \nabla\cdot\left(\frac{\alpha_a^n}{B_a^{n+1}}\nabla(\rho_a^{n+1} g D)\right)\right) = 0 \qquad (3.3)$$

The functions p_{ca} and p_{cv} is assumed to be a function of S_a, S_v respectively. Thus we have the following relation

$$\nabla p_{ca} = p'_{ca}(S_a)\nabla S_a, \quad \text{and} \quad \nabla p_{cv} = p'_{cv}(S_v)\nabla S_v. \qquad (3.4)$$

Using the above equation, (3.3) can be rewritten as

$$\frac{1}{\Delta t}((\phi S_a)^{n+1} - (\phi S_a)^n) + \left(\phi S_a\left(-\frac{1}{B_a}\frac{dB_a}{dp}\right)\right)^{n+1}\frac{p^{n+1}-p^n}{\Delta t}$$
$$-B_a^{n+1}\left(\nabla\cdot\left(\frac{\alpha_a^n}{B_a^{n+1}}p'_{ca}(S_a^n)\nabla S_a^{n+1}\right)\right) - B_a^{n+1}\left(\nabla\cdot\left(\frac{\alpha_a^n}{B_a^{n+1}}\nabla(p^{n+1}-\rho_a^{n+1}gD)\right)\right) \tag{3.5}$$

Now we are ready to discretize (3.1), (3.2) and (3.5) in space using the DG method. Denote $\mathcal{L}_1 := (3.1)$, we can simplify the equation by writing

$$\begin{aligned}\mathcal{L}_1(p,S_L,S_a) &= A^n\left(\frac{p^{n+1}-p^n}{\Delta t}\right) - \sum_{i=1}^{4} b_i^n\nabla\cdot(c_i^n\nabla p^{n+1}) + y^n(p_{cv},p_{ca}) \\ &\quad + \sum_{i=1}^{4} d_i^n\nabla\cdot(f_i^n\nabla(h_i^n gD)),\end{aligned} \tag{3.6}$$

where

$$\begin{aligned}A &= \phi^o c_R + \phi^o(1+c_R(p-p^o))\Big(c_L S_L(1+R_{sL})^{-1}\Big(1+R_{sL}+\frac{S_aB_L}{B_aS_L}+\frac{S_vB_L}{B_vS_L}\Big) \\ &\quad + c_vS_v\Big(1+\frac{B_vR_{sL}S_L}{B_LS_v}+\frac{B_vS_a}{B_aS_v}+\frac{S_LB_v}{B_LS_v}\Big)+c_aS_a\Big(1+\frac{B_aS_L}{B_LS_a}+\frac{B_a}{S_a}\Big(\frac{S_v}{B_v}+\frac{S_LR_{sL}}{B_L}\Big)\Big)\Big),\end{aligned} \tag{3.7}$$

and

$$y = -B_v\nabla\cdot(\frac{\alpha_v}{B_v}\nabla p_{cv}) - B_a\nabla\cdot(\frac{\alpha_a}{B_a}\nabla p_{ca}), \tag{3.8}$$

and the values of b_i, c_i, d_i, f_i, h_i for $i = 1,\ldots,4$ are shown in Table 3.1.

Let Ω be a bounded domain in $\Re^d$ where $d = 2,3$ and $\mathcal{E} = \{E\}_h$ be a mesh of Ω. Suppose $\mathcal{D}(\mathcal{E}_h) = \{v : v|_E \in P_k(E), \forall E \in \mathcal{E}_h\}$ where $P_k(E)$ denotes the space of polynomials with total polynomial degree k on element E. Let $k_p^E, k_{s_L}^E, k_{s_a}^E$ represent the polynomial degree on E for the approximation of p, S_L, S_a respectively. Then we define

$$\begin{aligned}k_p &= \max\{k_p^E : E\in\mathcal{E}_h\}, \\ k_{s_i} &= \max\{k_{s_i}^E : E\in\mathcal{E}_h\} \quad \text{for } i = a, L.\end{aligned}$$

Table 3.1 : Coefficients of $\mathcal{L}_1(p, S_L, S_a)$

i	b_i	c_i	d_i	f_i	h_i
1	$B_L - B_v R_{sL}$	$\frac{\alpha_L}{B_L}$	$B_L - B_v R_{sL}$	$\frac{\alpha_L}{B_L}$	ρ_L
2	B_v	$\frac{\alpha_v}{B_v}$	B_v	$\frac{\alpha_v}{B_v}$	ρ_v
3	B_v	$\frac{R_{sL}\alpha_L}{B_L}$	B_a	$\frac{\alpha_a}{B_a}$	ρ_a
4	B_a	$\frac{\alpha_a}{B_a}$	B_v	$R_{sL}\frac{\alpha_L}{B_L}$	ρ_L

Let Γ_h be the set of interior edges of elements of $\mathcal{E}_h$. We denote an edge by e and associate with it a unit normal vector $\boldsymbol{n}_e$ directed from element E^m to E^n with $m > n$. Under this orientation, we define jump and average of a function Φ on e by:

$$\text{Jump of } \Phi : [\Phi] = (\Phi|_{E^m})_e - (\Phi|_{E^n})_e$$
$$\text{Average of } \Phi : \{\Phi\} = \frac{(\Phi|_{E^m})_e + (\Phi|_{E^n})_e}{2}$$

Multiplying $\mathcal{L}_1(p, S_L, S_a)$ by $v \in \mathcal{D}(\mathcal{E}_h)$, integrating over one mesh element and summing over all elements gives:

$$\sum_{E\in\mathcal{E}_h} \left(A^n \left(\frac{p^{n+1} - p^n}{\Delta t} \right), v \right)_E - \sum_{i=1}^{4} \left(\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} b_i^n \nabla \cdot (c_i^n \nabla p^{n+1}) v \right)$$
$$+ \sum_{E\in\mathcal{E}_h} (y^n, v)_E + \sum_{i=1}^{4} \left(\sum_{E\in\mathcal{E}_h} (d_i^n \nabla \cdot f_i^n \nabla (h_i^n g D), v)_E \right) = 0. \tag{3.9}$$

Notice one can evaluate the following integral using Green's theorem. If $\boldsymbol{n}_E$ is the outward normal to E, then one obtains the following expression:

$$\begin{aligned}
\int_{E\in\mathcal{E}_h} b_i\nabla\cdot(c_i\nabla p)v &= \int_{E\in\mathcal{E}_h} \nabla\cdot(c_i\nabla p)(b_iv) \\
&= -\int_{E\in\mathcal{E}_h} c_i\nabla p\cdot\nabla(b_iv) + \int_{\partial E} c_i\nabla p\cdot \boldsymbol{n}_E b_iv \\
&= -\int_{E\in\mathcal{E}_h} c_i\nabla p\cdot(b_i\nabla v + v\nabla b_i) + \int_{\partial E} c_i\nabla p\cdot \boldsymbol{n}_E b_iv \\
&= -\int_{E\in\mathcal{E}_h} c_ib_i\nabla p\cdot\nabla v - \int_{E\in\mathcal{E}_h} c_iv\nabla p\cdot\nabla b_i \\
&\quad + \int_{\partial E} c_i\nabla p\cdot \boldsymbol{n}_E b_iv. \qquad (3.10)
\end{aligned}$$

Here we write

$$\begin{aligned}
\sum_{E\in\mathcal{E}_h}\int_{\partial E} c_i\nabla p\cdot\boldsymbol{n}_E b_iv &= \sum_{E\in\mathcal{E}_h}\int_{\partial E} b_ic_i\nabla p\cdot\boldsymbol{n}_E v \\
&= \sum_{e\in\Gamma_h}\int_e\{b_ic_i\nabla p\cdot\boldsymbol{n}_e\}[v] - \epsilon\sum_{e\in\Gamma_h}\int_e\{b_ic_i\nabla v\cdot\boldsymbol{n}_e\}[p] \\
&\quad -\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p][v] \qquad (3.11)
\end{aligned}$$

where $\epsilon = \{-1, 1\}$. If we choose $\epsilon = 1$, we arrive at a non-symmetric interior Galerkin method (NIPG). If ϵ is equal to -1, we obtain a symmetric interior Galerkin method (SIPG). From the above equations, we obtain the following numerical scheme:

Suppose $(p^n, s_L^n, s_a^n) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_L}}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_a}}(\mathcal{E}_h)$ is known, find $(p^{n+1}, s_L^{n+1}, s_a^{n+1}) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_L}}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_a}}(\mathcal{E}_h)$ such that for all test function $(v, w, z) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_L}}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{s_a}}(\mathcal{E}_h)$, the following system is satisfied.

Pressure Equation

$$\sum_{E\in\mathcal{E}_h}\left(A^n\left(\frac{p^{n+1}-p^n}{\triangle t}\right),v\right)_E+\sum_{i=1}^{4}\Big(\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}c_i^n b_i^n\nabla p^{n+1}\cdot\nabla v$$
$$+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}c_i^n v\nabla p^{n+1}\cdot\nabla b_i^n-\sum_{e\in\Gamma_h}\int_e\{b_i^n c_i^n\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]$$
$$+\epsilon\sum_{e\in\Gamma_h}\int_e\{b_i^n c_i^n\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]\Big)+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]$$
$$+\sum_{E\in\mathcal{E}_h}(y^n,v)_E+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}(d_i^n\nabla\cdot f_i^n\nabla(h_i^n gD),v)_E=0. \tag{3.12}$$

We denote the saturation equations as $\mathcal{L}_2 := (3.2)$ and $\mathcal{L}_3 := (3.5)$. Similarly, we discretize $\mathcal{L}_2$ and $\mathcal{L}_3$ and obtain:

Saturation Equation for phase L

$$\sum_{E\in\mathcal{E}_h}\left(\frac{(\phi S_L)^{n+1}-(\phi S_L)^n}{\triangle t},w\right)_E+\sum_{E\in\mathcal{E}_h}\left(\phi^{n+1}S_L^{n+1}\left(-\frac{1}{B_L}\frac{dB_L}{dp}\right)^{n+1}\frac{p^{n+1}-p^n}{\triangle t},w\right)_E$$
$$+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_L^n}{B_L^{n+1}}\nabla p^{n+1}\cdot(B_L^{n+1}\nabla w+w\nabla B_L^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_L^n\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[w]+\underbrace{\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_L^n\nabla w\cdot\boldsymbol{n}_e\}[p^{n+1}]}_{:=1}$$
$$+\underbrace{\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][w]}_{:=2}-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_L^n}{B_L^{n+1}}\nabla(\rho_L^{n+1}gD)\cdot(B_L^{n+1}\nabla w+w\nabla B_L^{n+1})$$
$$+\sum_{e\in\Gamma_h}\int_e\{\alpha_L^n\nabla(\rho_L^{n+1}gD)\cdot\boldsymbol{n}_e\}[w]-\underbrace{\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_L^n\nabla w\cdot\boldsymbol{n}_e\}[\rho_L gD]}_{:=3}$$
$$-\underbrace{\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[\rho_L gD][w]}_{:=4}=0. \tag{3.13}$$

and

Saturation Equation for phase a

$$\sum_{E\in\mathcal{E}_h}\left(\frac{(\phi S_a)^{n+1}-(\phi S_a)^n}{\Delta t},z\right)_E+\sum_{E\in\mathcal{E}_h}\left(\left(\phi S_a\left(-\frac{1}{B_a}\frac{dB_a}{dp}\right)\right)^{n+1}\frac{p^{n+1}-p^n}{\Delta t},z\right)_E$$
$$+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^n}{B_a^{n+1}}p'_{ca}(S_a^n)\nabla S_a^{n+1}\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n p'_{ca}(S_a^n)\nabla S_a^{n+1}\cdot\boldsymbol{n}_e\}[z]+\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n p'_{ca}(S_a^n)\nabla z\cdot\boldsymbol{n}_e\}[S_a^{n+1}]$$
$$+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[S_a^{n+1}][z]+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^n}{B_a^{n+1}}\nabla p^{n+1}\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[z]+\underbrace{\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n\nabla z\cdot\boldsymbol{n}_e\}[p]}_{:=5}+\underbrace{\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p][z]}_{:=6}$$
$$-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^n}{B_a^{n+1}}\nabla(\rho_a^{n+1}gD)\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$+\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n\nabla(\rho_a^{n+1}gD)\cdot\boldsymbol{n}_e\}[z]-\underbrace{\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^n\nabla z\cdot\boldsymbol{n}_e\}[\rho_a^{n+1}gD]}_{:=7}$$
$$-\underbrace{\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[\rho_a^{n+1}gD][z]}_{:=8}=0. \tag{3.14}$$

Note that (1,2,3,4,5,6,7,8) are the stabilization terms for the DG scheme, but it might not be necessary to include them for convergency of the method. The reason is that the terms (1,2,3,4) does not associate with the primary unknown, here it is S_L, corresponding to the saturation equation for phase L. The same reasoning holds for terms (5,6,7,8). To find out if these terms are required, one can test it through numerical implementation.

3.2 Fully Coupled Formulation for Saturated Black Oil Model

Replace all the functions that are dependent on S_a, S_L and evaluate them at $n+1$, then we obtain a system of nonlinear equations:

Pressure Equation

$$\sum_{E\in\mathcal{E}_h}\left(A^{n+1}\left(\frac{p^{n+1}-p^n}{\triangle t}\right),v\right)_E+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h}c_i^{n+1}b_i^{n+1}\nabla p^{n+1}\cdot\nabla v$$
$$+\int_{E\in\mathcal{E}_h}c_i^{n+1}v\nabla p^{n+1}\cdot\nabla b_i^{n+1}-\sum_{e\in\Gamma_h}\int_e\{b_i^{n+1}c_i^{n+1}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]$$
$$+\epsilon\sum_{e\in\Gamma_h}\int_e\{b_i^{n+1}c_i^{n+1}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]\Big)+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]+\sum_{E\in\mathcal{E}_h}(y^{n+1},v)_E$$
$$+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}(d_i^{n+1}\nabla\cdot f_i^{n+1}\nabla(h_i^{n+1}gD),v)_E=0. \tag{3.15}$$

Saturation Equation for phase L

$$\sum_{E\in\mathcal{E}_h}\left(\frac{(\phi S_L)^{n+1}-(\phi S_L)^n}{\triangle t},w\right)_E+\sum_{E\in\mathcal{E}_h}\left(\phi^{n+1}S_L^{n+1}\left(-\frac{1}{B_L}\frac{dB_L}{dp}\right)^{n+1}\frac{p^{n+1}-p^n}{\triangle t},w\right)_E$$
$$+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_L^{n+1}}{B_L^{n+1}}\nabla p^{n+1}\cdot(B_L^{n+1}\nabla w+w\nabla B_L^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_L^{n+1}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[w]+\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_L^{n+1}\nabla w\cdot\boldsymbol{n}_e\}[p^{n+1}]$$
$$+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][w]-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_L^{n+1}}{B_L^{n+1}}\nabla(\rho_L^{n+1}gD)\cdot(B_L^{n+1}\nabla w+w\nabla B_L^{n+1})$$
$$+\sum_{e\in\Gamma_h}\int_e\{\alpha_L^{n+1}\nabla(\rho_L^{n+1}gD)\cdot\boldsymbol{n}_e\}[w]-\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_L^{n+1}\nabla w\cdot\boldsymbol{n}_e\}[\rho_L^{n+1}gD]$$
$$-\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[\rho_L^{n+1}gD][w]=0. \tag{3.16}$$

Saturation Equation for phase a

$$\sum_{E\in\mathcal{E}_h}\Big(\frac{(\phi S_a)^{n+1}-(\phi S_a)^n}{\Delta t},z\Big)_E+\sum_{E\in\mathcal{E}_h}\Big(\Big(\phi S_a\Big(-\frac{1}{B_a}\frac{dB_a}{dp}\Big)\Big)^{n+1}\frac{p^{n+1}-p^n}{\Delta t},z\Big)_E$$
$$+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^{n+1}}{B_a^{n+1}}p'_{ca}(S_a^{n+1})\nabla S_a^{n+1}\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}p'_{ca}(S_a^{n+1})\nabla S_a^{n+1}\cdot\boldsymbol{n}_e\}[z]+\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}\nabla z^{n+1}\cdot\boldsymbol{n}_e\}[p_{ca}]$$
$$+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p_{ca}][z]+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^{n+1}}{B_a^{n+1}}\nabla p^{n+1}\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$-\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[z]+\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}\nabla z\cdot\boldsymbol{n}_e\}[p]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p][z]$$
$$-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a^{n+1}}{B_a^{n+1}}\nabla(\rho_a gD)\cdot(B_a^{n+1}\nabla z+z\nabla B_a^{n+1})$$
$$+\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}\nabla(\rho_a gD)\cdot\boldsymbol{n}_e\}[z]-\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a^{n+1}\nabla z\cdot\boldsymbol{n}_e\}[\rho_a gD]$$
$$-\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[\rho_a gD][z]=0. \tag{3.17}$$

Now we define $L_4 := (3.15)$, $L_5 := (3.16)$,$L_6 := (3.17)$. Applying the Newton-Raphson method with $(\xi^0,\chi^0,\eta^0)=(p^n,S_L^n,S_a^n)$, the Newton iterates are defined by the following system:

$$\begin{pmatrix}\xi^{l+1}\\ \chi^{l+1}\\ \eta^{l+1}\end{pmatrix}=\begin{pmatrix}\xi^{l}\\ \chi^{l}\\ \eta^{l}\end{pmatrix}-\begin{pmatrix}\frac{dL_4}{dp^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_4}{dS_a^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_4}{dS_L^{n+1}}(\xi^l,\chi^l,\eta^l)\\ \frac{dL_5}{dp^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_5}{dS_a^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_5}{dS_L^{n+1}}(\xi^l,\chi^l,\eta^l)\\ \frac{dL_6}{dp^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_6}{dS_a^{n+1}}(\xi^l,\chi^l,\eta^l) & \frac{dL_6}{dS_L^{n+1}}(\xi^l,\chi^l,\eta^l)\end{pmatrix}^{-1}\begin{pmatrix}L_4(\xi^l,\chi^l,\eta^l)\\ L_5(\xi^l,\chi^l,\eta^l)\\ L_6(\xi^l,\chi^l,\eta^l)\end{pmatrix}$$

(3.18)

We now present an algorithm for the solution of the pressure, saturation equation.

Algorithm

1. Fix $\epsilon > 0$. Input initial values with $(\xi^0, \chi^0, \eta^0) = (p^n, S_a^n, S_L^n)$.

2. For $l = 0, 1, \ldots,$ do

   (a) Compute $\xi^{l+1}, \chi^{l+1}, \eta^{l+1}$ by solving (3.18).

   (b) If $||\xi^{l+1} - \xi^l||_{L^2(\Omega)} < \epsilon$, $||\chi^{l+1} - \chi^l||_{L^2(\Omega)} < \epsilon$ and $||\eta^{l+1} - \eta^l||_{L^2(\Omega)} < \epsilon$, return $l = l_*$ and stop.

3. Let $p^{n+1} = \xi^{l_*}$, $S_a^{n+1} = \chi^{l_*}$, $S_L^{n+1} = \eta^{l_*}$.

Here the pressure p is written in the following form:

$$p = \sum_{E\in\mathcal{E}_h} \sum_{j=1} a_{j,E}\psi_{j,E}(x,y), \tag{3.19}$$

where $\psi_{j,E}$ represents the set of basis over E and $a_{j,E}$ is the coefficient corresponding to $\psi_{j,E}$. To assemble the Jacobian J of (3.18) the entries of J are computed. For simplicity, we drop the index $n+1$ from now on.

$$\begin{aligned}\frac{\partial \mathcal{L}_4}{\partial p} \;=\;& \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{vp}{\Delta t}\frac{\partial A}{\partial p} + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{vA}{\Delta t}\frac{\partial p}{\partial p} - \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \left(\frac{p^n v}{\Delta t}\right) \underbrace{\frac{\partial A}{\partial p}}_{:=\spadesuit} \\ &+ \sum_{i=1}^{4} \Big(\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} c_i \frac{\partial b_i}{\partial p} \nabla p \cdot \nabla v + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} b_i \frac{\partial c_i}{\partial p} \nabla p \cdot \nabla v \\ &+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} c_i b_i \frac{\partial(\nabla p)}{\partial p} \cdot \nabla v + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} v \frac{\partial c_i}{\partial p} \nabla p \cdot \nabla b_i\end{aligned} \tag{3.20}$$

$$
\begin{aligned}
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} c_i v\frac{\partial}{\partial p}(\nabla p\cdot\nabla b_i)-\sum_{e\in\Gamma_h}\int_e\frac{\partial}{\partial p}\{b_ic_i\nabla p\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\Big(\Big\{\frac{\partial(b_ic_i)}{\partial p}\nabla v\cdot\boldsymbol{n}_e\Big\}[p]\ +\{b_ic_i\nabla v\cdot\boldsymbol{n}_e\}\frac{\partial[p]}{\partial p}\Big)\Big)\\
&+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[v]\frac{\partial[p]}{\partial p}+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial y}{\partial p}v\\
&+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h} v\frac{\partial d_i}{\partial p}(\nabla\cdot f_i\nabla(h_igD))\\
&+\int_{E\in\mathcal{E}_h} d_iv\frac{\partial}{\partial p}(\nabla\cdot f_i\nabla(h_igD))\Big)
\end{aligned}
\tag{3.21}
$$

Note that the term $\dfrac{\partial p}{\partial p}$ is kept due to the fact that the partial derivative with respect to p corresponds to the partial derivative with respect to $a_{j,E}$. Therefore, depending on the element E that we are taking the derivative of, we cannot simply write $\dfrac{\partial p}{\partial p}=1$. Now we compute $\dfrac{\partial\mathcal{L}_4}{\partial S_L}$, which is given by:

$$
\begin{aligned}
\frac{\partial\mathcal{L}_4}{\partial S_L} \;=\;& \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{(p-p^n)v}{\Delta t}\frac{\partial A}{\partial S_L}+\sum_{i=1}^{4}\Big(\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} b_i\frac{\partial c_i}{\partial S_L}\nabla p\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} c_i\frac{\partial b_i}{\partial S_L}\nabla p\cdot\nabla v+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} v\frac{\partial c_i}{\partial S_L}\nabla p\cdot\nabla b_i\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} c_iv\nabla p\cdot\frac{\partial(\nabla b_i)}{\partial S_L}-\sum_{e\in\Gamma_h}\int_e[v]\Big\{\frac{\partial(b_ic_i)}{\partial S_L}\nabla p\cdot\boldsymbol{n}_e\Big\}\\
&+\epsilon\sum_{e\in\Gamma_h}\int_{\partial E}\Big\{\frac{\partial(b_ic_i)}{\partial S_L}\nabla v\cdot\boldsymbol{n}_e\Big\}[p]\Big)\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial y}{\partial S_L}v+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h} v\frac{\partial d_i}{\partial S_L}(\nabla\cdot f_i\nabla(h_igD))\\
&+\int_{E\in\mathcal{E}_h} d_iv(\nabla\cdot\frac{\partial f_i}{\partial S_L}\nabla(h_igD))\Big)
\end{aligned}
\tag{3.22}
$$

The calcuation of $\dfrac{\partial \mathcal{L}_4}{\partial S_a}$ is the same as $\dfrac{\partial \mathcal{L}_4}{\partial S_L}$, replace S_L by S_a.

$$
\begin{aligned}
\frac{\partial \mathcal{L}_4}{\partial S_a} &= \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{(p-p^n)v}{\triangle t}\frac{\partial A}{\partial S_a}+\sum_{i=1}^{4}\Big(\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} b_i\frac{\partial c_i}{\partial S_a}\nabla p\cdot\nabla v \\
&\quad +\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} c_i\frac{\partial b_i}{\partial S_a}\nabla p\cdot\nabla v+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} v\frac{\partial c_i}{\partial S_a}\nabla p\cdot\nabla b_i \\
&\quad +\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} c_i v\nabla p\cdot\frac{\partial(\nabla b_i)}{\partial S_a}-\sum_{e\in\Gamma_h}\int_e [v]\Big\{\frac{\partial(b_ic_i)}{\partial S_a}\nabla p\cdot\boldsymbol{n}_e\Big\} \\
&\quad +\epsilon\sum_{e\in\Gamma_h}\int_{\partial E}\Big\{\frac{\partial(b_ic_i)}{\partial S_a}\nabla v\cdot\boldsymbol{n}_e\Big\}[p]\Big) \\
&\quad +\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial y}{\partial S_a}v+\sum_{i=1}^{4}\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h} v\frac{\partial d_i}{\partial S_a}(\nabla\cdot f_i\nabla(h_i gD)) \\
&\quad +\int_{E\in\mathcal{E}_h} d_i v(\nabla\cdot\frac{\partial f_i}{\partial S_a}\nabla(h_i gD))\Big)
\end{aligned}
\tag{3.23}
$$

Now we compute $\dfrac{\partial \mathcal{L}_5}{\partial \beta_i}$ with $\beta=(p,S_L,S_a)$, then we obtain:

$$
\begin{aligned}
\frac{\partial \mathcal{L}_5}{\partial p} &= \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\phi^o c_R\frac{wS_L}{\triangle t}\frac{\partial p}{\partial p}+\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h} S_L\frac{(p-p^n)w}{\triangle t}\frac{\partial}{\partial p}\Big(-\frac{\phi}{B_L}\frac{\partial B_L}{\partial p}\Big) \\
&\quad +\int_{E\in\mathcal{E}_h}\frac{w}{\triangle t}\frac{\partial p}{\partial p}\Big(-\frac{\phi S_L}{B_L}\frac{\partial B_L}{\partial p}\Big)\Big)+\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h}\frac{1}{B_L}\frac{\partial \alpha_L}{\partial p}\nabla p\cdot(B_L\nabla w+w\nabla B_L) \\
&\quad -\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L^2}\frac{\partial B_L}{\partial p}\nabla p\cdot(B_L\nabla w+w\nabla B_L)+\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L}\frac{\partial}{\partial p}(\nabla p\cdot(B_L\nabla w)) \\
&\quad +\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L}\frac{\partial}{\partial p}(\nabla p\cdot(w\nabla B_L))\Big)-\sum_{e\in\Gamma_h}\int_e\Big\{\frac{\partial(\alpha_L\nabla p)}{\partial p}\cdot\boldsymbol{n}_e\Big\}[w] \\
&\quad +\epsilon\sum_{e\in\Gamma_h}\Big(\int_e\Big\{\frac{\partial \alpha_L}{\partial p}\nabla w\cdot\boldsymbol{n}_e\Big\}[p]+\int_e\{\alpha_L\nabla w\cdot\boldsymbol{n}_e\}\frac{\partial[p]}{\partial p}\Big)
\end{aligned}
\tag{3.24}
$$

$$+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[p]}{\partial p}[w]-\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h}\frac{1}{B_L}\frac{\partial\alpha_L}{\partial p}\nabla(\rho_L gD)\cdot(B_L\nabla w+w\nabla B_L)$$
$$+\sum_{E\in\mathcal{E}_h}\Big(\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L^2}\frac{\partial B_L}{\partial p}\nabla(\rho_L gD)\cdot(B_L\nabla w+w\nabla B_L)$$
$$-\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L}\frac{\partial}{\partial p}(\nabla(\rho_L gD)\cdot(B_L\nabla w))-\int_{E\in\mathcal{E}_h}\frac{\alpha_L}{B_L}\frac{\partial}{\partial p}(\nabla(\rho_L gD)\cdot(w\nabla B_L))\Big)$$
$$+\sum_{e\in\Gamma_h}\int_e[w]\frac{\partial}{\partial p}\{\alpha_L\nabla(\rho_L gD)\cdot\boldsymbol{n}_e\}-\epsilon\sum_{e\in\Gamma_h}\Big(\int_e\Big\{\frac{\partial\alpha_L}{\partial p}\nabla w\cdot\boldsymbol{n}_e\Big\}[\rho_L gD]\Big)$$
$$+\int_e\{\alpha_L\nabla w\cdot\boldsymbol{n}_e\}\frac{\partial[\rho_L]}{\partial p}gD-\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[\rho_L]}{\partial p}gD[w] \qquad (3.25)$$

and

$$\begin{aligned}\frac{\partial\mathcal{L}_5}{\partial S_L} &= \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\phi w}{\Delta t}\frac{\partial S_L}{\partial S_L}+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\phi\left(-\frac{1}{B_L}\frac{\partial B_L}{\partial p}\right)\frac{(p-p^n)w}{\Delta t}\frac{\partial S_L}{\partial S_L}\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial\alpha_L}{\partial S_L}\frac{\nabla p\cdot(B_L\nabla w+w\nabla B_L)}{B_L}\\
&-\sum_{e\in\Gamma_h}\int_e[w]\Big\{\frac{\partial\alpha_L}{\partial S_L}\nabla p\cdot\boldsymbol{n}_e\Big\}+\epsilon\sum_{e\in\Gamma_h}\int_e[p]\Big\{\frac{\partial\alpha_L}{\partial S_L}\nabla w\cdot\boldsymbol{n}_e\Big\}\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial\alpha_L}{\partial S_L}\frac{\nabla(\rho_L gD)\cdot(B_L\nabla w+w\nabla B_L)}{B_L}\\
&+\sum_{e\in\Gamma_h}\int_e\Big\{\frac{\partial\alpha_L}{\partial S_L}\nabla(\rho_L gD)\cdot\boldsymbol{n}_e\Big\}[w]-\epsilon\sum_{e\in\Gamma_h}\int_e\Big\{\frac{\partial\alpha_L}{\partial S_L}\nabla w\cdot\boldsymbol{n}_e\Big\}[\rho_L gD]\end{aligned} \qquad (3.26)$$

and

$$\begin{aligned}\frac{\partial\mathcal{L}_5}{\partial S_a} &= \int_{E\in\mathcal{E}_h}\frac{\partial\alpha_L}{\partial S_a}\left(\frac{1}{B_L}\nabla p\cdot(B_L\nabla w+w\nabla B_L)\right)\\
&-\sum_{e\in\Gamma_h}\int_e[w]\Big\{\frac{\partial\alpha_L}{\partial S_a}\nabla p\cdot\boldsymbol{n}_e\Big\}+\epsilon\sum_{e\in\Gamma_h}\int_e[p]\Big\{\frac{\partial\alpha_L}{\partial S_a}\nabla w\cdot\boldsymbol{n}_e\Big\}\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial\alpha_L}{\partial S_a}\left(\frac{1}{B_L}\nabla(\rho_L gD)\cdot(B_L\nabla w+w\nabla B_L)\right)\\
&+\sum_{e\in\Gamma_h}\int_e[w]\Big\{\frac{\partial\alpha_L}{\partial S_a}\nabla(\rho_L gD)\cdot\boldsymbol{n}_e\Big\}-\epsilon\sum_{e\in\Gamma_h}\int_e[\rho_L gD]\Big\{\frac{\partial\alpha_L}{\partial S_a}\nabla w\cdot\boldsymbol{n}_e\Big\}.\end{aligned} \qquad (3.27)$$

Next, we continue computing the remaining entries of the Jacobian matrix and arrive at:

$$
\begin{aligned}
\frac{\partial \mathcal{L}_6}{\partial p} = & \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \phi^o c_R \frac{zS_a}{\triangle t}\frac{\partial p}{\partial p} - \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{(p-p^n)z}{\triangle t}\frac{\phi^o c_R S_a}{B_a}\frac{\partial B_a}{\partial p} \\
& - \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{(p-p^n)z}{\triangle t}\frac{\phi S_a}{B_a}\frac{\partial^2 B_a}{\partial p^2} + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{(p-p^n)z}{\triangle t}\frac{\phi S_a}{B_a^2}\Big(\frac{\partial B_a}{\partial p}\Big)^2 \\
& + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{z\phi S_a}{\triangle t}\frac{\partial p}{\partial p}\left(-\frac{1}{B_a}\frac{\partial B_a}{\partial p}\right) \\
& + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{1}{B_a}\frac{\partial \alpha_a}{\partial p}(p'_{ca}(S_a)\nabla S_a\cdot(B_a\nabla z + z\nabla B_a)) \\
& - \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{\alpha_a}{B_a^2}\frac{\partial B_a}{\partial p}(p'_{ca}(S_a)\nabla S_a\cdot(B_a\nabla z + z\nabla B_a)) \\
& + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{\alpha_a}{B_a}\Big(p'_{ca}(S_a)\nabla S_a\cdot\Big(\frac{\partial B_a}{\partial p}\nabla z + z\frac{\partial(\nabla B_a)}{\partial p}\Big)\Big) \\
& - \sum_{e\in\Gamma_h}\int_e [z]\frac{\partial}{\partial p}\{\alpha_a p'_{ca}(S_a)\nabla S_a\cdot\boldsymbol{n}_e\} + \epsilon\sum_{e\in\Gamma_h}\int_e [p_{ca}]\frac{\partial}{\partial p}\{\alpha_a\nabla z\cdot\boldsymbol{n}_e\} \\
& + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e \frac{\partial[p_{ca}]}{\partial p}[z] \\
& + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{1}{B_a}\frac{\partial \alpha_a}{\partial p}(\nabla p\cdot(B_a\nabla z + z\nabla B_a)) \\
& - \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{\alpha_a}{B_a^2}\frac{\partial B_a}{\partial p}(\nabla p\cdot(B_a\nabla z + z\nabla B_a)) \\
& + \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h} \frac{\alpha_a}{B_a}\frac{\partial}{\partial p}(\nabla p\cdot(B_a\nabla z + z\nabla B_a)) \\
& - \sum_{e\in\Gamma_h}\int_e [z]\frac{\partial}{\partial p}\{\alpha_a\nabla p\cdot\boldsymbol{n}_e\} + \epsilon\sum_{e\in\Gamma_h}\int_e \Big\{\frac{\partial \alpha_a}{\partial p}\nabla z\cdot\boldsymbol{n}_e\Big\}[p] \\
& + \epsilon\sum_{e\in\Gamma_h}\int_e \{\alpha_a\nabla z\cdot\boldsymbol{n}_e\}\frac{\partial[p]}{\partial p} + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e \frac{\partial[p]}{\partial p}[z]
\end{aligned} \tag{3.28}
$$

$$
\begin{aligned}
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{B_a}\frac{\partial\alpha_a}{\partial p}(\nabla(\rho_a gD)\cdot(B_a\nabla z+z\nabla B_a))\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a}{B_a^2}\frac{\partial B_a}{\partial p}(\nabla(\rho_a gD)\cdot(B_a\nabla z+z\nabla B_a))\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a}{B_a}\frac{\partial}{\partial p}(\nabla(\rho_a gD)\cdot(B_a\nabla z))\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\alpha_a}{B_a}\frac{\partial}{\partial p}(\nabla(\rho_a gD)\cdot(z\nabla B_a))\\
&+\sum_{e\in\Gamma_h}\int_e[z]\frac{\partial}{\partial p}\{\alpha_a\nabla(\rho_a gD)\cdot\boldsymbol{n}_e\}-\epsilon\sum_{e\in\Gamma_h}\int_e[\rho_a gD]\left\{\frac{\partial\alpha_a}{\partial p}\nabla z\cdot\boldsymbol{n}_e\right\}\\
&-\epsilon\sum_{e\in\Gamma_h}\int_e\frac{\partial[\rho_a]}{\partial p}gD\{\alpha_a\nabla z\cdot\boldsymbol{n}_e\}-\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[\rho_a]}{\partial p}gD[z]. \qquad (3.29)
\end{aligned}
$$

Note that $\mathcal{L}_6$ is a function independent of S_L, so we obtain

$$
\frac{\partial\mathcal{L}_6}{\partial S_L} = 0. \qquad (3.30)
$$

Now we compute $\dfrac{\partial\mathcal{L}_6}{\partial S_a}$, which is:

$$
\begin{aligned}
\frac{\partial\mathcal{L}_6}{\partial S_a} = &\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\phi z}{\Delta t}\frac{\partial S_a}{\partial S_a}+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\phi\left(-\frac{1}{B_a}\frac{dB_a}{dp}\right)\frac{p-p^n}{\Delta t}\frac{\partial S_a}{\partial S_a}z\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{B_a}\frac{\partial}{\partial S_a}\left(\alpha_a p'_{ca}(S_a)\nabla S_a\right)\cdot(B_a\nabla z+z\nabla B_a)\\
&-\sum_{e\in\Gamma_h}\int_e[z]\frac{\partial}{\partial S_a}\{\alpha_a p'_{ca}(S_a)\nabla S_a\cdot\boldsymbol{n}_e\}+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{\frac{\partial\alpha_a}{\partial S_a}\nabla z\cdot\boldsymbol{n}_e\right\}[p_{ca}]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{\alpha_a\nabla z\cdot\boldsymbol{n}_e\}\frac{\partial[p_{ca}]}{\partial S_a}+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[p_{ca}]}{\partial S_a}[z]
\end{aligned}
\qquad (3.31)
$$

$$
\begin{aligned}
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial\alpha_a}{\partial S_a}\frac{\nabla p}{B_a}\cdot(B_a\nabla z+z\nabla B_a)\\
&-\sum_{e\in\Gamma_h}\int_e[z]\Big\{\frac{\partial\alpha_a}{\partial S_a}\nabla p\cdot\boldsymbol{n}_e\Big\}+\epsilon\sum_{e\in\Gamma_h}\int_e[p]\Big\{\frac{\partial\alpha_a}{\partial S_a}\nabla z\cdot\boldsymbol{n}_e\Big\}\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\partial\alpha_a}{\partial S_a}\frac{\nabla(\rho_a gD)}{B_a}\cdot(B_a\nabla z+z\nabla B_a)\\
&+\sum_{e\in\Gamma_h}\int_e[z]\Big\{\frac{\partial\alpha_a}{\partial S_a}\nabla(\rho_a gD)\cdot\boldsymbol{n}_e\Big\}-\epsilon\sum_{e\in\Gamma_h}\int_e[\rho_a gD]\Big\{\frac{\partial\alpha_a}{\partial S_a}\nabla z\cdot\boldsymbol{n}_e\Big\}.
\end{aligned}
\tag{3.32}
$$

From (♠), we calculate

$$
\begin{aligned}
\frac{\partial A}{\partial p} \;=\;& \phi^o c_R\frac{\partial p}{\partial p}\Big(c_L S_L(1+R_{sL})^{-1}\Big(1+R_{sL}+\frac{S_aB_L}{B_aS_L}+\frac{S_vB_L}{B_vS_L}\Big)+c_vS_v\Big(1+\frac{B_vR_{sL}S_L}{B_LS_v}\\
&+\frac{B_vS_a}{B_aS_v}+\frac{S_LB_v}{B_LS_v}\Big)+c_aS_a\Big(1+\frac{B_aS_L}{B_LS_a}+\frac{B_a}{S_a}\Big(\frac{S_v}{B_v}+\frac{S_LR_{sL}}{B_L}\Big)\Big)\Big)\\
&+\phi^o(1+c_R(p-p^o))\Big(S_L(1+R_{sL})^{-1}\frac{\partial c_L}{\partial p}\Big(1+R_{sL}+\frac{S_aB_L}{B_aS_L}+\frac{S_vB_L}{B_vS_L}\Big)\\
&-\frac{S_Lc_L}{(1+R_{sL})^2}\frac{\partial R_{sL}}{\partial p}\Big(1+R_{sL}+\frac{S_aB_L}{B_aS_L}+\frac{S_vB_L}{B_vS_L}\Big)\\
&+c_LS_L(1+R_{sL})^{-1}\Big(\frac{\partial R_{sL}}{\partial p}+\frac{S_a}{S_L}\frac{\partial}{\partial p}\Big(\frac{B_L}{B_a}\Big)+\frac{S_v}{S_L}\frac{\partial}{\partial p}\Big(\frac{B_L}{B_v}\Big)\Big)\\
&+S_v\frac{\partial c_v}{\partial p}\Big(1+\frac{B_vR_{sL}S_L}{B_LS_v}+\frac{B_vS_a}{B_aS_v}+\frac{S_LB_v}{B_LS_v}\Big)\\
&+S_vc_v\Big(\frac{S_L}{S_v}\frac{\partial}{\partial p}\Big(\frac{B_vR_{sL}}{B_L}\Big)+\frac{S_a}{S_v}\frac{\partial}{\partial p}\Big(\frac{B_v}{B_a}\Big)+\frac{S_L}{S_v}\frac{\partial}{\partial p}\Big(\frac{B_v}{B_L}\Big)\Big)\\
&+S_a\frac{\partial c_a}{\partial p}\Big(1+\frac{B_aS_L}{B_LS_a}+\frac{B_a}{S_a}\Big(\frac{S_v}{B_v}+\frac{S_LR_{sL}}{B_L}\Big)\Big)\\
&+S_ac_a\Big(\frac{S_L}{S_a}\frac{\partial}{\partial p}\Big(\frac{B_a}{B_L}\Big)+\frac{S_v}{S_a}\frac{\partial}{\partial p}\Big(\frac{B_a}{B_v}\Big)+\frac{S_L}{S_a}\frac{\partial}{\partial p}\Big(\frac{B_aR_{sL}}{B_L}\Big)\Big)\Big).
\end{aligned}
\tag{3.33}
$$

Subsequently, from (3.7) we have

$$\begin{aligned}
\frac{\partial A}{\partial S_L} &= \phi^o(1+c_R(p-p^o))\Big(c_L(1+R_{sL})^{-1}\frac{\partial S_L}{\partial S_L}\Big(1+R_{sL}+\frac{S_aB_L}{B_aS_L}+\frac{S_vB_L}{B_vS_L}\Big) \\
&\quad -c_LS_L(1+R_{sL})^{-1}\Big(\frac{B_L}{B_a}\frac{S_a}{S_L^2}+\frac{B_L}{B_v}\frac{S_L+S_v}{S_L^2}\Big) \\
&\quad -c_v\frac{\partial S_L}{\partial S_L}\Big(1+\frac{B_vR_{sL}}{B_L}\frac{S_L}{S_v}+\frac{B_v}{B_a}\frac{S_a}{S_v}+\frac{S_L}{B_L}\frac{B_v}{S_v}\Big) \\
&\quad +c_vS_v\Big(\frac{B_vR_{sL}}{B_L}\frac{S_v+S_L}{S_v^2}+\frac{B_v}{B_a}\frac{S_a}{S_v^2}+\frac{B_v}{B_L}\frac{S_v+S_L}{S_v^2}\Big) \\
&\quad +c_aS_a\Big(\frac{1}{S_a}\frac{B_a}{B_L}-\frac{1}{S_a}\frac{B_a}{B_v}+\frac{1}{S_a}\frac{B_aR_{sL}}{B_L}\Big)\Big),
\end{aligned} \tag{3.34}$$

and

$$\begin{aligned}
\frac{\partial A}{\partial S_a} &= \phi^o(1+c_R(p-p^o))\Big(c_LS_L(1+R_{sL})^{-1}\Big(\frac{B_L}{B_a}\frac{1}{S_L}+\frac{B_L}{B_v}\frac{-S_L+S_v}{S_L^2}\Big) \\
&\quad -c_v\frac{\partial S_a}{\partial S_a}\Big(1+\frac{B_vR_{sL}}{B_L}\frac{S_L}{S_v}+\frac{B_v}{B_a}\frac{S_a}{S_v}+\frac{S_L}{B_L}\frac{B_v}{S_v}\Big) \\
&\quad +c_vS_v\Big(\frac{B_vR_{sL}}{B_L}\frac{S_L}{S_v^2}+\frac{B_v}{B_a}\frac{S_a}{S_v^2}+\frac{B_v}{B_L}\frac{S_L}{S_v^2}\Big) \\
&\quad +c_a\frac{\partial S_a}{\partial S_a}\Big(1+\frac{B_aS_L}{B_LS_a}+\frac{B_a}{S_a}\Big(\frac{S_v}{B_v}+\frac{S_LR_{sL}}{B_L}\Big)\Big) \\
&\quad -c_aS_a\Big(\frac{B_a}{B_L}\frac{S_L}{S_a^2}+\frac{B_a}{B_v}\frac{S_a+S_v}{S_a^2}+\frac{B_aR_{sL}}{B_L}\frac{S_L}{S_a^2}\Big)\Big).
\end{aligned} \tag{3.35}$$

Now from (3.8), we compute:

$$\begin{aligned}
\frac{\partial y}{\partial p} &= \frac{\partial}{\partial p}\Big(B_v\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_{cv}\Big)+B_a\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_{ca}\Big)\Big) \\
&= \frac{\partial B_v}{\partial p}\nabla\cdot\Big(\frac{\alpha_v}{B_v}\nabla p_{cv}\Big)+B_v\nabla\cdot\Big(\frac{\partial}{\partial p}\Big(\frac{\alpha_v}{B_v}\Big)\nabla p_{cv}\Big) \\
&\quad +\frac{\partial B_a}{\partial p}\nabla\cdot\Big(\frac{\alpha_a}{B_a}\nabla p_{ca}\Big)+B_a\nabla\cdot\Big(\frac{\partial}{\partial p}\Big(\frac{\alpha_a}{B_a}\Big)\nabla p_{ca}\Big)
\end{aligned} \tag{3.36}$$

Using the form of p given by (3.19), we see that $\dfrac{\partial}{\partial p}(\nabla p\cdot\nabla v)$ is given by

$$\begin{aligned}
\frac{\partial}{\partial a_{j,E}}(\nabla p\cdot\nabla v) &= \frac{\partial(\nabla p)}{\partial a_{j,E}}\cdot\nabla v \\
&= \nabla\psi_{j,E}(x,y)\cdot\nabla v.
\end{aligned} \tag{3.37}$$

Table 3.2 : Table of partial derivatives of b_i with respect to p, S_L, S_a

	$\frac{\partial b_i}{\partial p}$	$\frac{\partial b_i}{\partial S_\alpha}$ for $\alpha = L, a$
$i = 1$	$\frac{\partial B_L}{\partial p} - R_{sL}\frac{\partial B_v}{\partial p} - B_v\frac{\partial R_{sL}}{\partial p}$	0
$i = 2$	$\frac{\partial B_v}{\partial p}$	0
$i = 3$	$\frac{\partial B_v}{\partial p}$	0
$i = 4$	$\frac{\partial B_a}{\partial p}$	0

Table 3.3 : Table of partial derivatives of c_i with respect to p, S_L, S_a

	$\frac{\partial c_i}{\partial p}$	$\frac{\partial c_i}{\partial S_\alpha}$ for $\alpha = L, a$
$i = 1$	$-\frac{k_{rL}\mathbf{k}}{B_L^2\mu_L}\frac{\partial B_L}{\partial p} - \frac{k_{rL}\mathbf{k}}{B_L\mu_L^2}\frac{\partial \mu_L}{\partial p}$	$\frac{\mathbf{k}}{B_L\mu_L}\frac{\partial k_{rL}}{\partial S_\alpha}$
$i = 2$	$-\frac{k_{rv}\mathbf{k}}{B_v^2\mu_v}\frac{\partial B_v}{\partial p} - \frac{k_{rv}\mathbf{k}}{B_v\mu_v^2}\frac{\partial \mu_v}{\partial p}$	$\frac{\mathbf{k}}{B_L\mu_v}\frac{\partial k_{rv}}{\partial S_\alpha}$
$i = 3$	$\frac{k_{rL}\mathbf{k}}{B_L\mu_L}\frac{\partial R_{sL}}{\partial p} - \frac{R_{sL}k_{rL}\mathbf{k}}{B_L\mu_L^2}\frac{\partial \mu_L}{\partial p} - \frac{R_{sL}k_{rL}\mathbf{k}}{B_L^2\mu_L}\frac{\partial B_L}{\partial p}$	$\frac{R_{sL}\mathbf{k}}{B_L\mu_L}\frac{\partial k_{rL}}{\partial S_\alpha}$
$i = 4$	$-\frac{k_{ra}\mathbf{k}}{B_a\mu_a^2}\frac{\partial \mu_a}{\partial p} - \frac{k_{ra}\mathbf{k}}{B_a^2\mu_a}\frac{\partial B_a}{\partial p}$	$\frac{\mathbf{k}}{B_a\mu_a}\frac{\partial k_{ra}}{\partial S_\alpha}$

Table 3.4 : Table of partial derivatives of d_i with respect to p, S_L, S_a

	$\frac{\partial d_i}{\partial p}$	$\frac{\partial d_i}{\partial S_\alpha}$ for $\alpha = L, a$
$i = 1$	$\frac{\partial B_L}{\partial p} - R_{sL}\frac{\partial B_v}{\partial p} - B_v\frac{\partial R_{sL}}{\partial p}$	0
$i = 2$	$\frac{\partial B_v}{\partial p}$	0
$i = 3$	$\frac{\partial B_a}{\partial p}$	0
$i = 4$	$\frac{\partial B_v}{\partial p}$	0

Table 3.5 : Table of partial derivatives of f_i with respect to p, S_L, S_a

	$\frac{\partial f_i}{\partial p}$	$\frac{\partial f_i}{\partial S_\alpha}$ for $\alpha = L, a$
$i = 1$	$-\frac{k_{rL}\mathbf{k}}{\mu_L^2 B_L}\frac{\partial \mu_L}{\partial p} - \frac{k_{rL}\mathbf{k}}{\mu_L B_L^2}\frac{\partial B_L}{\partial p}$	$\frac{\mathbf{k}}{\mu_L B_L}\frac{\partial k_{rL}}{\partial S_\alpha}$
$i = 2$	$-\frac{k_{rv}\mathbf{k}}{\mu_v^2 B_v}\frac{\partial \mu_v}{\partial p} - \frac{k_{rv}\mathbf{k}}{\mu_v B_v^2}\frac{\partial B_v}{\partial p}$	$\frac{\mathbf{k}}{\mu_v B_v}\frac{\partial k_{rv}}{\partial S_\alpha}$
$i = 3$	$-\frac{k_{ra}}{\mu_a^2 B_a}\frac{\partial \mu_a}{\partial p} - \frac{k_{ra}\mathbf{k}}{\mu_a B_a^2}\frac{\partial B_a}{\partial p}$	$\frac{\mathbf{k}}{\mu_a B_a}\frac{\partial k_{ra}}{\partial S_\alpha}$
$i = 4$	$\frac{k_{rL}\mathbf{k}}{\mu_L B_L}\frac{\partial R_{sL}}{\partial p} - \frac{k_{rL}\mathbf{k}}{\mu_L^2 B_L}\frac{\partial \mu_L}{\partial p} - \frac{k_{rL}\mathbf{k}}{\mu_L B_L^2}\frac{\partial B_L}{\partial p}$	$\frac{R_{sL}\mathbf{k}}{\mu_L B_L}\frac{\partial k_{rL}}{\partial S_\alpha}$

Similarly using (3.19), we have

$$\begin{aligned} \frac{\partial}{\partial a_{j,E}}(\nabla p \cdot \nabla b_i) &= \frac{\partial(\nabla p)}{\partial a_{j,E}} \cdot \nabla b_i + \nabla p \cdot \frac{\partial(\nabla b_i)}{\partial a_{j,E}} \\ &= \nabla \psi_{j,E}(x,y) \cdot \nabla b_i + \nabla p \cdot \frac{\partial}{\partial a_{j,E}}(b_i'(p)\nabla p) \\ &= \nabla \psi_{j,E}(x,y) \cdot \nabla b_i + \nabla p \cdot (b_i''(p)\psi_{j,E}\nabla p) \\ &\quad + \nabla p \cdot \left(b_i'(p)\frac{\partial(\nabla p)}{\partial a_{j,E}}\right) \end{aligned} \tag{3.38}$$

Also, one obtain

$$\frac{\partial \alpha_L}{\partial S_\alpha} = \frac{1}{\mu_L}\frac{\partial k_{rL}}{\partial S_\alpha}\mathbf{k} \qquad \text{for } \alpha = L, a \tag{3.39}$$

and

$$\frac{\partial \alpha_L}{\partial p} = -\frac{k_{rL}}{\mu_L^2}\frac{\partial \mu_L}{\partial p}\mathbf{k}. \tag{3.40}$$

Now we compute $\frac{\partial \alpha_a}{\partial S_\alpha}$ for $\alpha = L, a$ and arrive at:

$$\frac{\partial \alpha_a}{\partial S_L} = \frac{1}{\mu_a}\frac{\partial k_{ra}}{\partial S_L}\mathbf{k} = 0 \tag{3.41}$$

and

$$\frac{\partial \alpha_a}{\partial S_a} = \frac{1}{\mu_a}\frac{\partial k_{ra}}{\partial S_a}\mathbf{k} = \frac{k_{ra}'(S_a)}{\mu_a}\mathbf{k} \tag{3.42}$$

with

$$\frac{\partial \alpha_a}{\partial p} = -\frac{k_{ra}}{\mu_L^2}\frac{\partial \mu_a}{\partial p}\mathbf{k}. \tag{3.43}$$

In the next section, an investigation on the geological sequestration of CO_2 is presented. A DG scheme is developed.

3.3 Sequential Formulation for CO_2 Sequestration Model

The primary unknowns of the systems are pressure, saturations and mole fractions: $p, S_L, x_{H_2O,v}, x_{CO_2,L}$. We first solve for p, S_L and then we use (2.65), (2.66) to obtain $x_{H_2O,v}, x_{CO_2,L}$. Discretizing (2.57), (2.58) in time and time lagging the mole fractions, we obtain:

Pressure Equation

$$\begin{aligned}
&\frac{1}{\triangle t}\Big(\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{CO_2,L}\rho^n_L S^n_L + x^n_{CO_2,v}\rho^n_v(1-S^n_L))\\
&-\phi^o(1+c_R(p^n-p^o))(x^n_{CO_2,L}\rho^n_L S^n_L + x^n_{CO_2,v}\rho^n_v(1-S^n_L))\Big)\\
&\underbrace{-\nabla\cdot\Big(\Big(x^n_{CO_2,L}\rho^n_L\mathbf{k}\frac{k^n_{rL}}{\mu^n_L} + x^n_{CO_2,v}\rho^n_v\mathbf{k}\frac{k^n_{rv}}{\mu^n_v}\Big)\nabla p^{n+1}\Big)\Big)}_{:=9}\\
&-\nabla\cdot\Big(x^n_{CO_2,v}\rho^n_v\mathbf{k}\frac{k^n_{rv}}{\mu^n_v}p'_{cv}(1-S^n_L)\nabla S^n_L\Big) + x^n_{CO_2,L}\rho^n_L q^n_L + x^n_{CO_2,v}\rho^n_v q^n_v = 0
\end{aligned} \tag{3.44}$$

Saturation Equation

$$\begin{aligned}
&\frac{1}{\triangle t}\Big(\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho^{n+1}_L S^{n+1}_L + x^n_{H_2O,v}\rho^{n+1}_v(1-S^{n+1}_L))\\
&-\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho^{n+1}_L S^n_L + x^n_{H_2O,v}\rho^{n+1}_v(1-S^n_L))\Big)
\end{aligned}$$

$$= \nabla\cdot\left(\left(x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}} + x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\right)\nabla p^{n+1}\right) + \underbrace{\nabla\cdot\left(x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S^n_L)\nabla S^n_L\right)}_{:=10} - x^n_{H_2O,L}\rho_L^{n+1}q^n_L - x^n_{H_2O,v}\rho_v^{n+1}q^n_v \tag{3.45}$$

From Green's theorem, we obtain

$$\begin{aligned}\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\nabla\cdot\left(x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla p\right)v &= -\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla p\cdot\nabla v \\ &\quad+\sum_{E\in\mathcal{E}_h}\int_{\partial E}x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla p\cdot\boldsymbol{n}_E v \\ &= -\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla p\cdot\nabla v \\ &\quad+\sum_{e\in\Gamma_h}\int_e\{x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla p\cdot\boldsymbol{n}_e\}[v] \\ &\quad-\epsilon\sum_{e\in\Gamma_h}\int_e\{x_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\nabla v\cdot\boldsymbol{n}_e\}[p] \\ &\quad-\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p][v]\end{aligned} \tag{3.46}$$

Using the expression above and apply DG to the terms (9), (10) in the pressure and saturation equations, we arrive at the following numerical scheme.

Suppose $(p^n, S^n_L) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$ is known, find $(p^{n+1}, S^{n+1}_L) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$ such that for all test function $(v,w) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$, the following system is satisfied:

Pressure Equation

$$
\begin{aligned}
&\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{CO_2,L}\rho_L^{n+1}S_L^n+x^n_{CO_2,v}\rho_v^{n+1}(1-S_L^n))v\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n}-p^o))(x^n_{CO_2,L}\rho_L^{n}S_L^n+x^n_{CO_2,v}\rho_v^{n}(1-S_L^n))v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla S_L^n\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla S_L^n\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla v\cdot\boldsymbol{n}_e\}[S_L^n]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[S_L^n][v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]\\
&+\sum_{E\in\mathcal{E}_h}\left(x^n_{CO_2,L}\rho_L^{n+1}q_L^n,v\right)_E+\sum_{E\in\mathcal{E}_h}\left(x^n_{CO_2,v}\rho_v^{n+1}q_v^n,v\right)_E=0
\end{aligned}
\tag{3.47}
$$

Saturation Equation

$$
\begin{aligned}
&\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho_L^{n+1}S_L^{n+1}+x^n_{H_2O,v}\rho_v^{n+1}(1-S_L^{n+1}))v\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho_L^{n+1}S_L^{n}+x^n_{H_2O,v}\rho_v^{n+1}(1-S_L^{n}))v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\right\}[v]\\
&\underbrace{+\,\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k^n_{rL}}{\mu_L^{n+1}}\nabla v\cdot\boldsymbol{n}_e\right\}[p^{n+1}]}_{:=11}+\underbrace{\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]}_{:=12}\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla S_L^{n+1}\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla S_L^{n+1}\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}p'_{cv}(1-S_L^n)\nabla v\cdot\boldsymbol{n}_e\right\}[S_L^{n+1}]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[S_L^{n+1}][v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\right\}[v]\\
&\underbrace{+\,\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k^n_{rv}}{\mu_v^{n+1}}\nabla v\cdot\boldsymbol{n}_e\right\}[p^{n+1}]}_{:=13}\\
&+\sum_{E\in\mathcal{E}_h}\left(x^n_{H_2O,L}\rho_L^{n+1}q_L^n,v\right)_E+\sum_{E\in\mathcal{E}_h}\left(x^n_{H_2O,v}\rho_v^{n+1}q_v^n,v\right)_E=0 \qquad (3.48)
\end{aligned}
$$

Here the stability terms (11), (12) and (13) may not be needed to keep the numerical scheme stable; however, this can be checked through numerical testing. An illustration of how our sequential scheme is applied is shown in Figure 3.1.

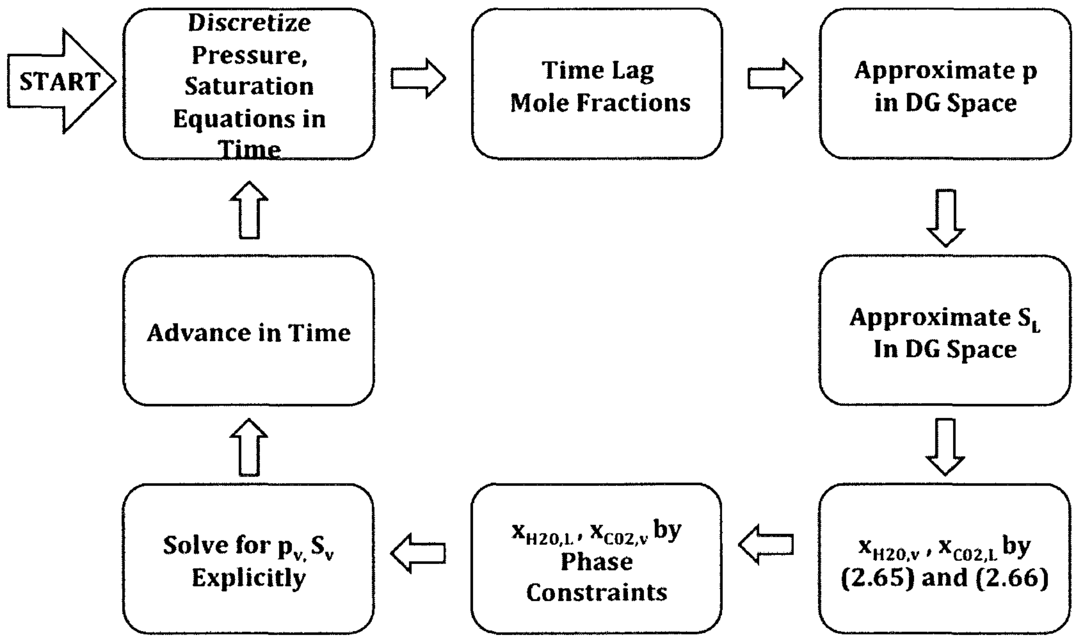

Figure 3.1 : Sequential Approach for the CO_2 Sequestration Model

3.4 Fully Coupled Formulation for CO_2 Sequestration Model

In this section we derive a fully coupled scheme to solve the CO_2 sequestration problem. First we discretize the coupled equations (2.57) and (2.58) in time, then we discretize this set of equations in DG space. The resulting pressure and saturation equations are similar to (3.47) and (3.48) where all the coefficients with subscript n replaced by $n+1$ with the exception of mole fractions.

Suppose $(p^n, S_L^n) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$ is known, find $(p^{n+1}, S_L^{n+1}) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$ such that for all test function $(v, w) \in \mathcal{D}_{k_p}(\mathcal{E}_h)$ x $\mathcal{D}_{k_{S_L}}(\mathcal{E}_h)$, the following system is satisfied:

Pressure Equation

$$\begin{aligned}
&\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{CO_2,L}\rho_L^{n+1}S_L^{n+1}+x^n_{CO_2,v}\rho_v^{n+1}(1-S_L^{n+1}))v\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{1}{\triangle t}\phi^o(1+c_R(p^{n}-p^o))(x^n_{CO_2,L}\rho_L^{n+1}S_L^{n+1}+x^n_{CO_2,v}\rho_v^{n+1}(1-S_L^{n+1}))v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla S_L^{n+1}\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla S_L^{n+1}\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla v\cdot\boldsymbol{n}_e\}[S_L^{n+1}]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[S_L^{n+1}][v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\nabla v-\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{CO_2,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}]\\
&+\sum_{E\in\mathcal{E}_h}\left(x^n_{CO_2,L}\rho_L^{n+1}q_L^{n+1},v\right)_E+\sum_{E\in\mathcal{E}_h}\left(x^n_{CO_2,v}\rho_v^{n+1}q_v^{n+1},v\right)_E=0 \qquad (3.49)
\end{aligned}$$

Saturation Equation

$$
\begin{aligned}
& \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{1}{\Delta t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho_L^{n+1}S_L^{n+1}+x^n_{H_2O,v}\rho_v^{n+1}(1-S_L^{n+1}))v \\
& -\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{1}{\Delta t}\phi^o(1+c_R(p^{n+1}-p^o))(x^n_{H_2O,L}\rho_L^{n+1}S_L^{n}+x^n_{H_2O,v}\rho_v^{n+1}(1-S_L^{n}))v \\
& +\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\nabla v - \sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v] \\
& +\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,L}\rho_L^{n+1}\mathbf{k}\frac{k_{rL}^{n+1}}{\mu_L^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}] + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v] \\
& +\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla S_L^{n+1}\cdot\nabla v \\
& -\sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla S_L^{n+1}\cdot\boldsymbol{n}_e\}[v] \\
& +\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}p'_{cv}(1-S_L^{n+1})\nabla v\cdot\boldsymbol{n}_e\}[S_L^{n+1}] + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[S_L^{n+1}][v] \\
& +\sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\nabla v - \sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla p^{n+1}\cdot\boldsymbol{n}_e\}[v] \\
& +\epsilon\sum_{e\in\Gamma_h}\int_e\{x^n_{H_2O,v}\rho_v^{n+1}\mathbf{k}\frac{k_{rv}^{n+1}}{\mu_v^{n+1}}\nabla v\cdot\boldsymbol{n}_e\}[p^{n+1}] + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e[p^{n+1}][v] \\
= & -\sum_{E\in\mathcal{E}_h}\left(x^n_{H_2O,L}\rho_L^{n+1}q_L^{n+1},v\right)_E - \sum_{E\in\mathcal{E}_h}\left(x^n_{H_2O,v}\rho_v^{n+1}q_v^{n+1},v\right)_E \qquad (3.50)
\end{aligned}
$$

Here we denote $\mathcal{C}_1$:=(3.49), $\mathcal{C}_2$:=(3.50) with $\mathcal{C}=(\mathcal{C}_1(y),\mathcal{C}_2(y))^T$ and $y=(p,S_L)$. Our primary unknowns are pressure p^{n+1} and saturation S_L^{n+1}. Now we outline an algorithm for solving the system. Denote $(\varphi^0,\lambda^0)=(p^n,S_L^n)$

Algorithm

1. Fix $\epsilon>0$. Input initial values for $x^0_{CO_2,L}$ and $x^0_{H_2O,L}$, S_L^0, p_v^0

2. Solve for $x^0_{CO_2,v}$ and $x^0_{H_2O,L}$ by phase constraints:

$$
\begin{aligned}
x^0_{CO_2,L}+x^0_{H_2O,L} &= 1 \\
x^0_{CO_2,v}+x^0_{H_2O,v} &= 1.
\end{aligned}
$$

3. For $l = 0, 1, \ldots,$ do

   (a) Compute $\varphi^{l+1}, \lambda^{l+1}$ by solving $\mathcal{C}_1 = 0$ and $\mathcal{C}_2 = 0$ using Newton-Raphson's method.

   (b) If $||\varphi^{l+1} - \varphi^l||_{L^2(\Omega)} < \epsilon$ and $||\lambda^{l+1} - \lambda^l||_{L^2(\Omega)} < \epsilon$, return $l = l_*$ and stop.

   (c) Let $p^{n+1} = \varphi^{l_*}$, $S_L^{n+1} = \lambda^{l_*}$ where l_* as the last l.

   (d) Compute $x_{H_2O,v}^{n+1}, x_{CO_2,L}^{n+1}$ by (2.65), (2.66).

   (e) Compute $x_{H_2O,L}^{n+1}, x_{H_2O,v}^{n+1}$ by phase constraints.

Figure 3.2 shows the schematic procedure of the fully coupled technique.

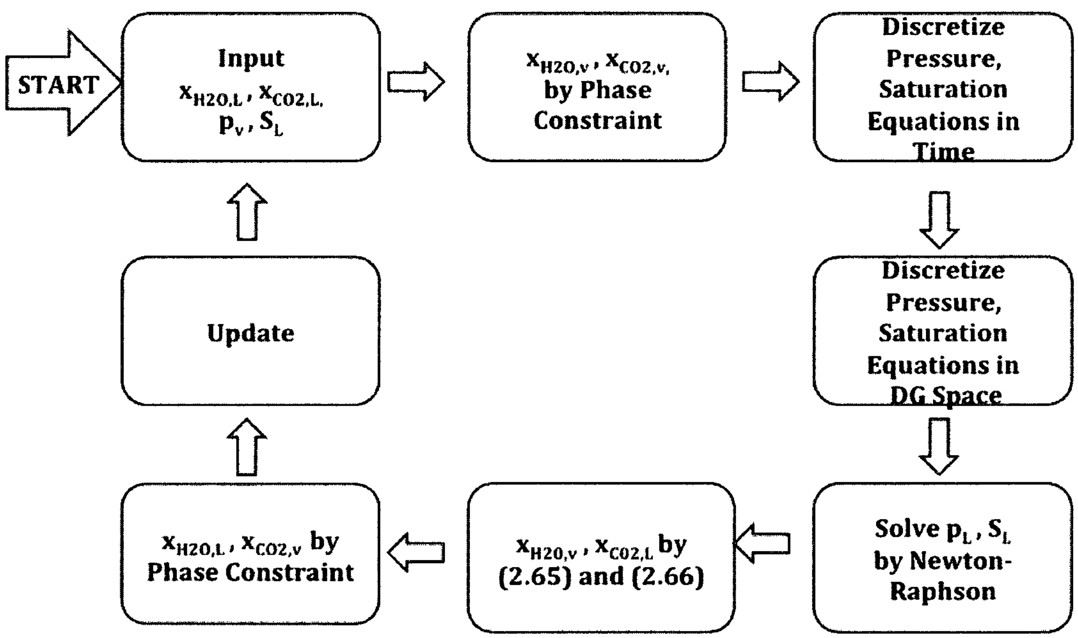

Figure 3.2 : Fully Coupled Approach for the CO_2 Sequestration Model

From the Newton-Raphson method, the entries of the Jacobian matrix are given by:

$$
\begin{aligned}
\frac{\partial \mathcal{C}_1}{\partial p} \quad = \quad & \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{v}{\triangle t}\phi^o c_R (x^n_{CO_2,L}\rho_L S_L + x^n_{CO_2,v}\rho_v(1-S_L))\frac{\partial p}{\partial p} \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{v}{\triangle t}\phi^o(1+c_R(p-p^o))\Big(x^n_{CO_2,L}S_L\frac{\partial \rho_L}{\partial p} + x_{CO_2,v}(1-S_L)\frac{\partial \rho_v}{\partial p}\Big) \\
& - \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{v}{\triangle t}\phi^o(1+c_R(p^n-p^o))\Big(x^n_{CO_2,L}S_L\frac{\partial \rho_L}{\partial p} + x_{CO_2,v}(1-S_L)\frac{\partial \rho_v}{\partial p}\Big) \\
& - \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{CO_2,L}k_{rL}\mathbf{k}\frac{\rho_L}{\mu_L^2}\frac{\partial \mu_L}{\partial p}\nabla p\cdot\nabla v \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{CO_2,L}k_{rL}}{\mu_L}\mathbf{k}\frac{\partial \rho_L}{\partial p}\nabla p\cdot\nabla v \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{CO_2,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\frac{\partial(\nabla p)}{\partial p}\cdot\nabla v \\
& - \sum_{e\in\Gamma_h} \int_e \Big\{x^n_{CO_2,L}k_{rL}\mathbf{k}\frac{\partial}{\partial p}\Big(\frac{\rho_L}{\mu_L}\nabla p\Big)\cdot\boldsymbol{n}_e\Big\}[v] \\
& +\epsilon\sum_{e\in\Gamma_h} \int_e \Big\{x^n_{CO_2,L}k_{rL}\mathbf{k}\frac{\partial}{\partial p}\Big(\frac{\rho_L}{\mu_L}\Big)\nabla v\cdot\boldsymbol{n}_e\Big\}[p] + \sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[p]}{\partial p}[v] \\
& - \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{CO_2,v}k_{rv}p'_{cv}(1-S_L)\mathbf{k}\frac{\rho_v}{\mu_v^2}\frac{\partial \mu_v}{\partial p}\nabla S_L\cdot\nabla v \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{CO_2,v}k_{rv}}{\mu_v}p'_{cv}(1-S_L)\mathbf{k}\frac{\partial \rho_v}{\partial p}\nabla S_L\cdot\nabla v \\
& - \sum_{e\in\Gamma_h} \int_e \Big\{x^n_{CO_2,v}k_{rv}\mathbf{k}\frac{\partial}{\partial p}\Big(\frac{\rho_v}{\mu_v}\Big)p'_{cv}(1-S_L)\nabla S_L\cdot\boldsymbol{n}_e\Big\}[v] \\
& +\epsilon\sum_{e\in\Gamma_h} \int_e \Big\{x^n_{CO_2,v}k_{rv}\mathbf{k}\frac{\partial}{\partial p}\Big(\frac{\rho_v}{\mu_v}\Big)p'_{cv}(1-S_L)\nabla v\cdot\boldsymbol{n}_e\Big\}[S_L] \\
& - \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{CO_2,v}k_{rv}\mathbf{k}\frac{\rho_v}{\mu_v^2}\frac{\partial \mu_v}{\partial p}\nabla p\cdot\nabla v \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{CO_2,v}k_{rv}}{\mu_v}\mathbf{k}\frac{\partial \rho_v}{\partial p}\nabla p\cdot\nabla v \\
& + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{CO_2,v}\rho_v\mathbf{k}\frac{k_{rv}}{\mu_v}\frac{\partial(\nabla p)}{\partial p}\cdot\nabla v
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}k_{rv}\mathbf{k}\frac{\partial}{\partial p}\left(\frac{\rho_L}{\mu_v}\nabla p\right)\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}k_{rv}\mathbf{k}\frac{\partial}{\partial p}\left(\frac{\rho_L}{\mu_v}\right)\nabla v\cdot\boldsymbol{n}_e\right\}[p]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[p]}{\partial p}[v]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,L}\;q_L v\frac{\partial\rho_L}{\partial p}+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{CO_2,v}\;q_v v\frac{\partial\rho_v}{\partial p}
\end{aligned}
\tag{3.51}
$$

Now we calculate the partial derivative of $\mathcal{C}_2$ with respect to p.

$$
\begin{aligned}
\frac{\partial\mathcal{C}_2}{\partial p} \;=\;& \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{v}{\triangle t}\phi^o c_R(x^n_{H_2O,L}\rho_L S_L+x^n_{H_2O,v}\rho_v(1-S_L))\frac{\partial p}{\partial p}\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{v}{\triangle t}\phi^o(1+c_R(p-p^o))\left(x^n_{H_2O,L}S_L\frac{\partial\rho_L}{\partial p}+x_{H_2O,v}(1-S_L)\frac{\partial\rho_v}{\partial p}\right)\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{v}{\triangle t}\phi^o(1+c_R(p^n-p^o))\left(x^n_{H_2O,L}S_L\frac{\partial\rho_L}{\partial p}+x_{H_2O,v}(1-S_L)\frac{\partial\rho_v}{\partial p}\right)\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,L}k_{rL}\mathbf{k}\frac{\rho_L}{\mu_L^2}\frac{\partial\mu_L}{\partial p}\nabla p\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,L}k_{rL}}{\mu_L}\mathbf{k}\frac{\partial\rho_L}{\partial p}\nabla p\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,L}\rho_L\mathbf{k}\frac{k_{rL}}{\mu_L}\frac{\partial(\nabla p)}{\partial p}\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}k_{rL}\mathbf{k}\frac{\partial}{\partial p}\left(\frac{\rho_L}{\mu_L}\nabla p\right)\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}k_{rL}\mathbf{k}\frac{\partial}{\partial p}\left(\frac{\rho_L}{\mu_L}\right)\nabla v\cdot\boldsymbol{n}_e\right\}[p]+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[p]}{\partial p}[v]\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}x^n_{H_2O,v}k_{rv}p'_{cv}(1-S_L)\mathbf{k}\frac{\rho_v}{\mu_v^2}\frac{\partial\mu_v}{\partial p}\nabla S_L\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,v}k_{rv}}{\mu_v}p'_{cv}(1-S_L)\mathbf{k}\frac{\partial\rho_v}{\partial p}\nabla S_L\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}k_{rv}\mathbf{k}\frac{\partial}{\partial p}\left(\frac{\rho_v}{\mu_v}\right)p'_{cv}(1-S_L)\nabla S_L\cdot\boldsymbol{n}_e\right\}[v]
\end{aligned}
$$

$$
\begin{aligned}
&+\epsilon \sum_{e\in\Gamma_h} \int_e \Big\{ x^n_{H_2O,v} k_{rv} \mathbf{k} \frac{\partial}{\partial p}\Big(\frac{\rho_v}{\mu_v}\Big) p'_{cv}(1-S_L)\nabla v \cdot \boldsymbol{n}_e \Big\} [S_L] \\
&- \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,v} k_{rv} \mathbf{k} \frac{\rho_v}{\mu_v^2} \frac{\partial \mu_v}{\partial p} \nabla p \cdot \nabla v \\
&+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{H_2O,v} k_{rv}}{\mu_v} \mathbf{k} \frac{\partial \rho_v}{\partial p} \nabla p \cdot \nabla v \\
&+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,v} \rho_v \mathbf{k} \frac{k_{rv}}{\mu_v} \frac{\partial(\nabla p)}{\partial p} \cdot \nabla v \\
&- \sum_{e\in\Gamma_h} \int_e \Big\{ x^n_{H_2O,v} k_{rv} \mathbf{k} \frac{\partial}{\partial p}\Big(\frac{\rho_L}{\mu_v}\nabla p\Big) \cdot \boldsymbol{n}_e \Big\} [v] \\
&+\epsilon \sum_{e\in\Gamma_h} \int_e \Big\{ x^n_{H_2O,v} k_{rv} \mathbf{k} \frac{\partial}{\partial p}\Big(\frac{\rho_L}{\mu_v}\Big) \nabla v \cdot \boldsymbol{n}_e \Big\} [p] + \sum_{e\in\Gamma_h} \frac{\sigma}{|e|} \int_e \frac{\partial [p]}{\partial p} [v] \\
&+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,L}\, q_L v \frac{\partial \rho_L}{\partial p} + \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} x^n_{H_2O,v}\, q_v v \frac{\partial \rho_v}{\partial p}
\end{aligned} \tag{3.52}
$$

Next we compute $\dfrac{\partial \mathcal{C}_i}{\partial S_L}$ with $i = 1$, and obtain:

$$
\begin{aligned}
\frac{\partial \mathcal{C}_1}{\partial S_L} &= \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{\phi^o(1 + c_R(p - p^o))v}{\triangle t} \Big(x^n_{CO_2,L} \rho_L \frac{\partial S_L}{\partial S_L} - x^n_{CO_2,v} \rho_v \frac{\partial S_L}{\partial S_L} \Big) \\
&- \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{\phi^o(1 + c_R(p^n - p^o))v}{\triangle t} \Big(x^n_{CO_2,L} \rho_L \frac{\partial S_L}{\partial S_L} - x^n_{CO_2,v} \rho_v \frac{\partial S_L}{\partial S_L} \Big) \\
&+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{CO_2,L} \rho_L \mathbf{k}}{\mu_L} \frac{\partial k_{rL}}{\partial S_L} \nabla p \cdot \nabla v \\
&- \sum_{e\in\Gamma_h} \int_e \Big\{ x^n_{CO_2,L} \frac{\rho_L}{\mu_L} \mathbf{k} \frac{\partial k_{rL}}{\partial S_L} \nabla p \cdot \boldsymbol{n}_e \Big\} [v] \\
&+\epsilon \sum_{e\in\Gamma_h} \int_e \Big\{ x^n_{CO_2,L} \frac{\rho_L}{\mu_L} \mathbf{k} \frac{\partial k_{rL}}{\partial S_L} \nabla v \cdot \boldsymbol{n}_e \Big\} [p] \\
&+ \sum_{E\in\mathcal{E}_h} \int_{E\in\mathcal{E}_h} \frac{x^n_{CO_2,v} \rho_v \mathbf{k}}{\mu_v} \frac{\partial k_{rv}}{\partial S_L} p'_{cv}(1 - S_L) \nabla S_L \cdot \nabla v
\end{aligned}
$$

$$
\begin{aligned}
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{CO_2,v}\rho_v k_{rv}\mathbf{k}}{\mu_v}\frac{\partial}{\partial S_L}(p'_{cv}(1-S_L))\nabla S_L\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{CO_2,v}\rho_v k_{rv}\mathbf{k}}{\mu_v}p'_{cv}(1-S_L)\frac{\partial(\nabla S_L)}{\partial S_L}\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial}{\partial S_L}\Big(k_{rv}p'_{cv}(1-S_L)\nabla S_L\Big)\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial}{\partial S_L}\Big(k_{rv}p'_{cv}(1-S_L)\Big)\nabla v\cdot\boldsymbol{n}_e\right\}[S_L]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}\rho_v\mathbf{k}\frac{k_{rv}}{\mu_v}p'_{cv}(1-S_L)\nabla v\cdot\boldsymbol{n}_e\right\}\frac{\partial[S_L]}{\partial S_L}\\
&+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[S_L]}{\partial S_L}[v]+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{CO_2,v}\rho_v\mathbf{k}}{\mu_v}\frac{\partial k_{rv}}{\partial S_L}\nabla p\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial k_{rv}}{\partial S_L}\nabla p\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{CO_2,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial k_{rv}}{\partial S_L}\nabla v\cdot\boldsymbol{n}_e\right\}[p]
\end{aligned}
\tag{3.53}
$$

and

$$
\begin{aligned}
\frac{\partial\mathcal{C}_2}{\partial S_L} \;=\;& \sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\phi^o(1+c_R(p-p^o))v}{\triangle t}\Big(x^n_{H_2O,L}\rho_L\frac{\partial S_L}{\partial S_L}-x^n_{H_2O,v}\rho_v\frac{\partial S_L}{\partial S_L}\Big)\\
&-\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{\phi^o(1+c_R(p^n-p^o))v}{\triangle t}\Big(x^n_{H_2O,L}\rho_L\frac{\partial S_L}{\partial S_L}-x^n_{H_2O,v}\rho_v\frac{\partial S_L}{\partial S_L}\Big)\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,L}\rho_L\mathbf{k}}{\mu_L}\frac{\partial k_{rL}}{\partial S_L}\nabla p\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}\frac{\rho_L}{\mu_L}\mathbf{k}\frac{\partial k_{rL}}{\partial S_L}\nabla p\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,L}\frac{\rho_L}{\mu_L}\mathbf{k}\frac{\partial k_{rL}}{\partial S_L}\nabla v\cdot\boldsymbol{n}_e\right\}[p]\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,v}\rho_v\mathbf{k}}{\mu_v}\frac{\partial k_{rv}}{\partial S_L}p'_{cv}(1-S_L)\nabla S_L\cdot\nabla v
\end{aligned}
$$

$$
\begin{aligned}
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,v}\rho_v k_{rv}\mathbf{k}}{\mu_v}\frac{\partial}{\partial S_L}(p'_{cv}(1-S_L))\nabla S_L\cdot\nabla v\\
&+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,v}\rho_v k_{rv}\mathbf{k}}{\mu_v}p'_{cv}(1-S_L)\frac{\partial(\nabla S_L)}{\partial S_L}\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial}{\partial S_L}\Big(k_{rv}p'_{cv}(1-S_L)\nabla S_L\Big)\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial}{\partial S_L}\Big(k_{rv}p'_{cv}(1-S_L)\Big)\nabla v\cdot\boldsymbol{n}_e\right\}[S_L]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\rho_v\mathbf{k}\frac{k_{rv}}{\mu_v}p'_{cv}(1-S_L)\nabla v\cdot\boldsymbol{n}_e\right\}\frac{\partial[S_L]}{\partial S_L}\\
&+\sum_{e\in\Gamma_h}\frac{\sigma}{|e|}\int_e\frac{\partial[S_L]}{\partial S_L}[v]+\sum_{E\in\mathcal{E}_h}\int_{E\in\mathcal{E}_h}\frac{x^n_{H_2O,v}\rho_v\mathbf{k}}{\mu_v}\frac{\partial k_{rv}}{\partial S_L}\nabla p\cdot\nabla v\\
&-\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial k_{rv}}{\partial S_L}\nabla p\cdot\boldsymbol{n}_e\right\}[v]\\
&+\epsilon\sum_{e\in\Gamma_h}\int_e\left\{x^n_{H_2O,v}\frac{\rho_v}{\mu_v}\mathbf{k}\frac{\partial k_{rv}}{\partial S_L}\nabla v\cdot\boldsymbol{n}_e\right\}[p].
\end{aligned}
\tag{3.54}
$$

In the next chapter, concluding remarks of this study are given following a discussion of possible future extension to this work.

Chapter 4

Conclusion

In this thesis, two new high-order numerical schemes are proposed to solve the multicomponent multiphase flow in porous media that arises in the petroleum and environmental industries. Both sequential and fully coupled schemes are developed based on a discontinuous Galerkin approximation to solve the black oil and CO_2 sequestration model. So far there does not exist any numerical methods that solves this model using the DG method. For the CO_2 sequestration problem, while DG has been applied to solve the traditional conservation equations, much remains to be done in the issue regarding the treatment of mass transfer of CO_2 in water; thus, the schemes developed here takes this effect into account by using Sasaki's model.

For the sequential approach, the coupled nonlinear pressure and saturations equations are linearized by solving them sequentially and by time-lagging the nonlinear coefficients. This approach yields a relatively fast solution on a time step basis, but may exhibit stability problems when trying to approximate the saturations at each time step.

Now for the fully coupled approach, the Newton-Raphson method is applied to decouple the nonlinear system of equations. At each time step, a Jacobian matrix is constructed. This is shown in detail in Chapter 3. The advantage of this scheme is that no slope limiting techniques are required for stabilization of the system.

Future work includes implementation of the existing numerical methods developed in Chapter 3 and compare the resulting simulation model with TOUGH2, which is a general-purpose multiphase fluid flow simulator. Another future extension would be to incorporate the gravity effect in the CO_2 sequestration model and investigate automatic adaptivity on unstructured meshes to provide better efficient solutions with a lower computational cost. In addition, I would also like to give an estimation of the penalty parameters for the DG scheme so that the scheme remains stable and convergent.

Chapter 5

Notation

Note: $\alpha \in \{L, v, a\}$ and $m \in \{w, g, o\}$.

- B_α - Volume factor for phase α
- c_R - Rock compressibility
- c_α - Compressibility of phase α
- D - Depth of reservoir
- g - Gravitational constant
- $f_{m,\alpha}$ - Fugacity of component m in phase α
- $\mathbf{k}$ - Absolute permeability tensor
- $K_{m,t,p}$ - Thermodynamic equilibrium constant of component m at temperature t and pressure p
- $k_{r\alpha}$ - Relative permeability for phase α
- N_m - Amount of component m
- N_α - Amount of a given component in phase α
- p - Pressure
- $p_{c\alpha}$ - Capillary pressure of phase α

- p^o - Reference pressure
- R - Gas constant
- R_{sL} - Solution gas/liquid ratio
- S_α - Saturation of phase α
- $\boldsymbol{u}_\alpha$ - Phase velocity of phase α
- V_α - Volume of phase α
- $\bar{V}_m$ - Average partial molar volume of component m
- $V_{\alpha m}$ - Partial molar volume of phase α with respect to component m
- $x_{m,\alpha}$ - Mole fraction of component m in phase α
- ϕ - Porosity
- τ_m - Fugacity coefficient of component m
- Θ_m - Divergence of the flux of component m
- ν_α - Specific volume of phase α
- μ_α - Fluid viscosity of phase α
- ϕ^o - Reference porosity at p^o

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